

## Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA160RXA

PASSWORD:

LOGINID/PASSWORD REJECTED

The loginid and/or password sent to STN were invalid. You either typed them incorrectly, or line noise may have corrupted them.

Do you wish to retry the logon?

Enter choice (v/N) :

Do you wish to use the same loginid and password?

Enter choice (y/N) :

Enter new loginid (or press [Enter] for SSSBTA160BXA) :

Enter new loginid:

LOGINED.

LOGINID: SSSPTA1600RXA

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 FEB 25 CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered  
NEWS 4 FEB 28 PATDPAFULL - New display fields provide for legal status data from INPADOC  
NEWS 5 FEB 28 BABS - Current-awareness alerts (SDIs) available  
NEWS 6 FEB 28 MEDLINE/LMEDLINE reloaded  
NEWS 7 MAR 02 GBFULL: New full-text patent database on STN  
NEWS 8 MAR 03 REGISTRY/ZREGISTRY - Sequence annotations enhanced  
NEWS 9 MAR 03 MEDLINE file segment of TOXCENTER reloaded  
NEWS 10 MAR 22 KOREAPAT now updated monthly; patent information enhanced  
NEWS 11 MAR 22 Original IDE display format returns to REGISTRY/ZREGISTRY  
NEWS 12 MAR 22 PATDPASPC - New patent database available  
NEWS 13 MAR 22 REGISTRY/ZREGISTRY enhanced with experimental property tags

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

**NEWS HOURS STN Operating Hours Plus Help Desk Availability**

NEWS INTER General Internet Information

General Internet Information  
NEWS LOGIN Welcome Banner and News Items

NEWS PHONE Direct Dial and Telecommunication Network Access to STN

NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific

research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 15:22:16 ON 01 APR 2005

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:22:23 ON 01 APR 2005  
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 31 MAR 2005 HIGHEST RN 847735-80-2  
DICTIONARY FILE UPDATES: 31 MAR 2005 HIGHEST RN 847735-80-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

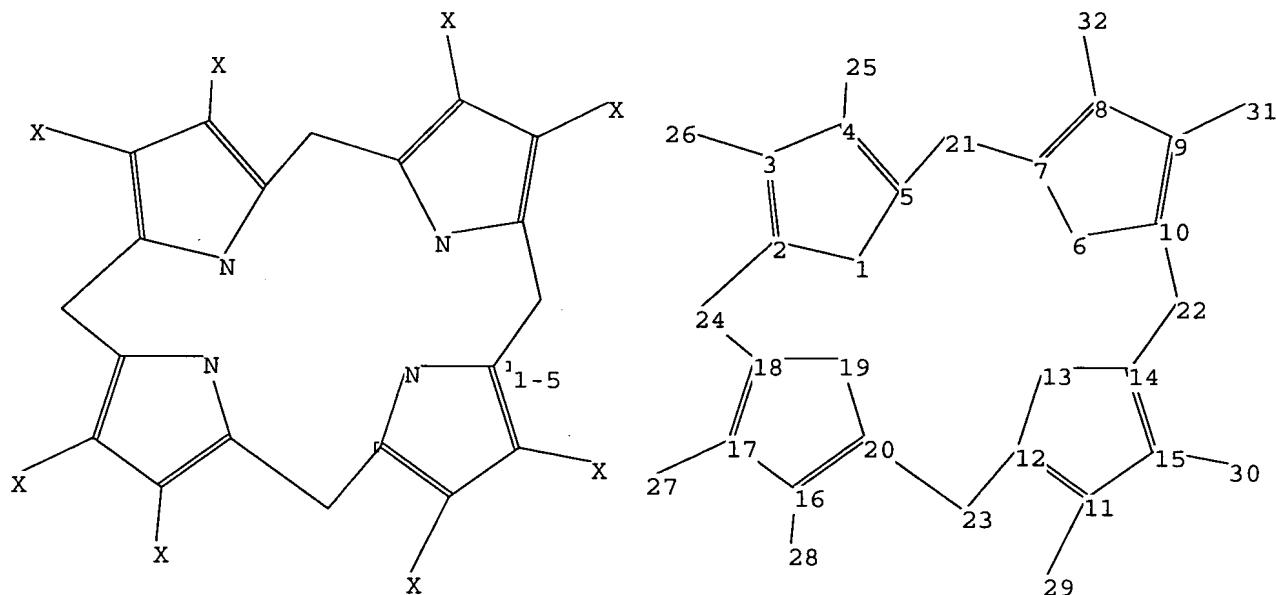
Please note that search-term pricing does apply when conducting SmartSELECT searches.

```
*****
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*****
```

Crossover limits have been increased. See **HELP CROSSOVER** for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> Uploading C:\Program Files\Stnexp\Queries\09939514.str

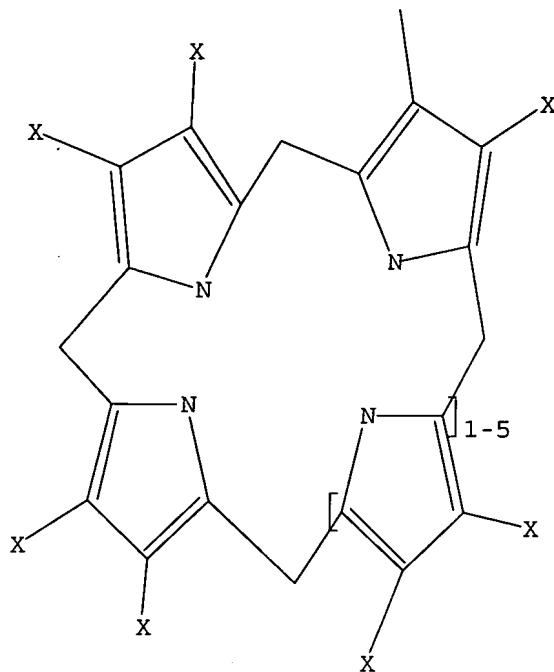


chain nodes :  
 25 26 27 28 29 30 31 32  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23  
 24  
 chain bonds :  
 3-26 4-25 8-32 9-31 11-29 15-30 16-28 17-27  
 ring bonds :  
 1-2 1-5 2-3 2-24 3-4 4-5 5-21 6-7 6-10 7-8 7-21 8-9 9-10 10-22 11-12  
 11-15 12-13 12-23 13-14 14-15 14-22 16-17 16-20 17-18 18-19 18-24 19-20  
 20-23  
 exact/norm bonds :  
 1-2 1-5 2-3 2-24 3-4 4-5 5-21 6-7 6-10 7-8 7-21 8-9 9-10 10-22 11-12  
 11-15 12-13 12-23 13-14 14-15 14-22 16-17 16-20 17-18 18-19 18-24 19-20  
 20-23  
 exact bonds :  
 3-26 4-25 8-32 9-31 11-29 15-30 16-28 17-27  
 isolated ring systems :  
 containing 1 :

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom  
 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS  
 29:CLASS 30:CLASS 31:CLASS 32:CLASS

L1 STRUCTURE UPLOADED

=> d  
 L1 HAS NO ANSWERS  
 L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11  
 SAMPLE SEARCH INITIATED 15:22:39 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 187 TO ITERATE

100.0% PROCESSED 187 ITERATIONS 11 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 2920 TO 4560  
 PROJECTED ANSWERS: 22 TO 418

L2 11 SEA SSS SAM L1

=> s 11 full  
 FULL SEARCH INITIATED 15:22:43 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 3675 TO ITERATE

100.0% PROCESSED 3675 ITERATIONS 127 ANSWERS  
 SEARCH TIME: 00.00.01

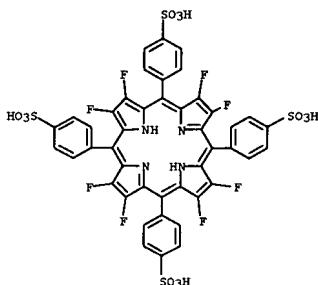
L3 127 SEA SSS FUL L1

=> s 13 and caplus/lc  
 45300192 CAPLUS/LC  
 L4 122 L3 AND CAPLUS/LC

=> s 13 not 14  
 L5 5 L3 NOT L4

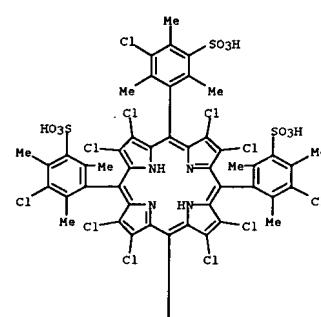
=> d 15 1-5

L5 ANSWER 1 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 756473-32-2 REGISTRY  
 ED Entered STN: 04 Oct 2004  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octafluoro-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis- (9CI) (CA INDEX NAME)  
 MF C44 H22 F8 N4 O12 S4  
 CI COM  
 SR CA

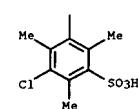


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 738554-86-4 REGISTRY  
 ED Entered STN: 03 Sep 2004  
 CN Benzenesulfonic acid, 3,3',3'',3'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[5-chloro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)  
 MF C56 H42 Cl12 N4 O12 S4  
 CI COM  
 SR CA

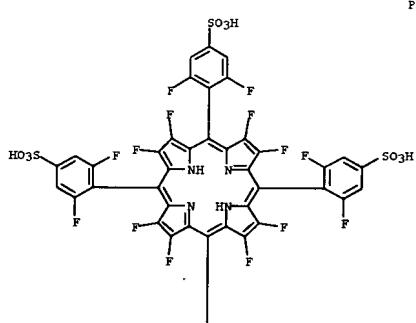


PAGE 1-A



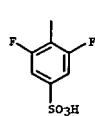
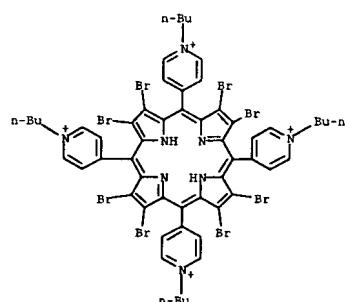
PAGE 2-A

L5 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 609215-74-5 REGISTRY  
 ED Entered STN: 03 Jun 2004  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octafluoro-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[3,5-difluoro- (9CI) (CA INDEX NAME)  
 MF C44 H14 F16 N4 O12 S4  
 CI COM  
 SR CA



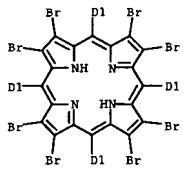
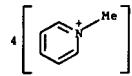
PAGE 1-A

L5 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN  
 RN 432028-74-5 REGISTRY  
 ED Entered STN: 19 Jun 2002  
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[1-butyl- (9CI) (CA INDEX NAME)  
 MF C56 H54 Br8 N8  
 CI COM  
 SR CA



PAGE 2-A

L5 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 206349-59-9 REGISTRY  
ED Entered STN: 04 Jun 1998  
CN Pyridinium, (2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[1-methyl- (9CI) (CA INDEX NAME)  
MF C44 H30 Br8 N8  
CI IDS, COM  
SR CA



=> fil caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY	SESSION
	175.99	176.20

FILE 'CAPLUS' ENTERED AT 15:24:00 ON 01 APR 2005  
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FILE COVERS 1907 - 1 Apr 2005 VOL 142 ISS 15  
 FILE LAST UPDATED: 31 Mar 2005 (20050331/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 15:22:16 ON 01 APR 2005)

FILE 'REGISTRY' ENTERED AT 15:22:23 ON 01 APR 2005  
 L1                   STRUCTURE UPLOADED  
 L2                   11 S L1  
 L3                   127 S L1 FULL  
 L4                   122 S L3 AND CAPLUS/LC  
 L5                   5 S L3 NOT L4

FILE 'CAPLUS' ENTERED AT 15:24:00 ON 01 APR 2005

=> s 14  
 L6                   148 L4

=> d ibib abs histr 16 1-148  
 'HISTR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB  
 ALL ----- BIB, AB, IND, RE  
 APPS ----- AI, PRAI  
 BIB ----- AN, plus Bibliographic Data and PI table (default)  
 CAN ----- List of CA abstract numbers without answer numbers  
 CBIB ----- AN, plus Compressed Bibliographic Data  
 DALL ----- ALL, delimited (end of each field identified)  
 DMAX ----- MAX, delimited for post-processing  
 FAM ----- AN, PI and PRAI in table, plus Patent Family data  
 FBIB ----- AN, BIB, plus Patent FAM

IND ----- Indexing data  
IPC ----- International Patent Classifications  
MAX ----- ALL, plus Patent FAM, RE  
PATS ----- PI, SO  
SAM ----- CC, SX, TI, ST, IT  
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;  
SCAN must be entered on the same line as the DISPLAY,  
e.g., D SCAN or DISPLAY SCAN)  
STD ----- BIB, IPC, and NCL

IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IMAX ----- MAX, indented with text labels  
ISTD ----- STD, indented with text labels

OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms  
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)  
containing hit terms  
HITRN ----- HIT RN and its text modification  
HITSTR ----- HIT RN, its text modification, its CA index name, and  
its structure diagram  
HITSEQ ----- HIT RN, its text modification, its CA index name, its  
structure diagram, plus NTE and SEQ fields  
FHITSTR ----- First HIT RN, its text modification, its CA index name, and  
its structure diagram  
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its  
structure diagram, plus NTE and SEQ fields  
KWIC ----- Hit term plus 20 words on either side  
OCC ----- Number of occurrence of hit term and field in which it occurs

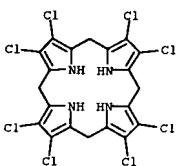
To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.

ENTER DISPLAY FORMAT (BIB):end

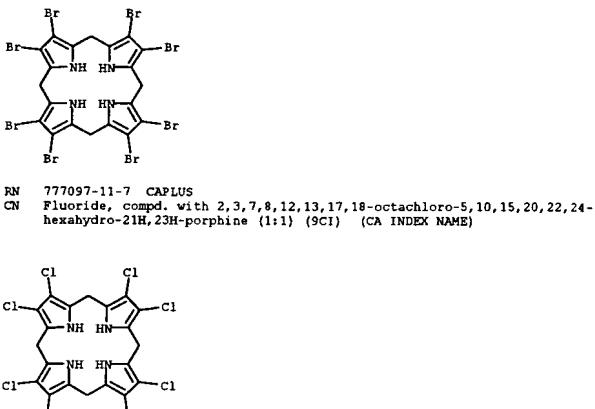
=> d ibib abs hitstr 1-148

L6 ANSWER 1 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:925092 CAPLUS  
 DOCUMENT NUMBER: 141:349685  
 TITLE: Density functional theory studies of  $\beta$ -substituent effect on conformational preference and anion binding ability of calix[4]pyrroles  
 AUTHOR(S): Wang, Di-Fei; Wu, Yundong  
 CORPORATE SOURCE: Department of Chemistry, The Hong Kong University of Science & Technology, Hong Kong, Peop. Rep. China  
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2004), (9), 96-110  
 CODEN: AGFUAR  
 URL: [http://www.arkat-usa.org/ark/journal/2004/109\\_Yua/n/CY-1155L/CY-1155L.pdf](http://www.arkat-usa.org/ark/journal/2004/109_Yua/n/CY-1155L/CY-1155L.pdf)  
 PUBLISHER: Arkat USA Inc.  
 DOCUMENT TYPE: Journal; (online computer file)  
 LANGUAGE: English  
 AB The conformational features and anion-binding properties of a series of  $\beta$ -octasubstituted calix[4]pyrroles have been investigated by the B3LYP method of d. functional theory with the 6-31+G\* basis set both in the gas phase and in CH2Cl2 solution. The calcns. demonstrated that adjusting the electronic properties of  $\beta$ -substituents on the pyrrole rings do change the anion-binding ability of calix[4]pyrroles. With the B3LYP/6-31+G\* method in CH2Cl2 solution, the relative binding energies follow the order of electron withdrawing abilities of the substituents, i.e. CN (18 kcal/mol) >> Cl (7 kcal/mol) > Br (4 kcal/mol) > H (0 kcal/mol). Calcns. also indicate that the energy difference between the most stable 1,3-alternate conformation and the least stable cone conformation that is for anion-binding is increased by electron-withdrawing  $\beta$ -substituents CN, Cl, and Br. Further anal. on dipyrromethane models reveals that the destabilization of the cone-conformation is mainly caused by electrostatic interactions between the  $\beta$ -substituents on the adjacent pyrrole rings. Our results thus provide useful information for designing stronger and more efficient calix[4]pyrrole-based anion binding receptors.  
 IT 777096-94-3 777096-95-4 777097-11-7  
 RL: PRP (Properties)  
 (DFT studies of  $\beta$ -substituent effect on conformational preference and anion binding ability of calix[4]pyrroles)  
 RN 777096-94-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20,22,24-hexahydro- (9CI) (CA INDEX NAME)



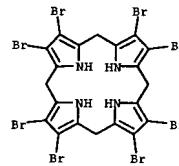
RN 777096-95-4 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro- (9CI) (CA INDEX NAME)

L6 ANSWER 1 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



● F-

RN 777097-12-8 CAPLUS  
 CN Fluoride, compd. with 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)



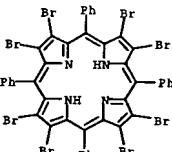
● F-

L6 ANSWER 1 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:598751 CAPLUS  
 DOCUMENT NUMBER: 141:266257  
 TITLE: Conformational analysis of octa- and tetrabromo tetraphenylporphyrins and their Ni(II) and Tb(III) complexes  
 AUTHOR(S): Gruden-Pavlovic, Maja; Grubisic, Sonja; Niketic, Svetozar R.  
 CORPORATE SOURCE: Belgrade, YU-11001, Journal of Inorganic Biochemistry (2004), 98(8), 1293-1302  
 SOURCE: CODEN: JIBIDJ; ISSN: 0162-0134  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Mol. mechanics (MM) calcns. were used to analyze the puckering of metalloporphyrins as a function of metal ion size and the position of substituents on the porphyrin periphery, on a three series of octa- and tetrabromo tetraphenylporphyrins: without metal, and with Ni(II), and Tb(III) as representative small and large metal ions, resp. Mol. energy optimization calcns. were carried out using the Consistent Force Field (CFF) program, with the parameters developed previously and new parameters for bromine atom. Normal-coordinate structural decomposition (NSD) anal. was performed on the equilibrium structures obtained by MM calcns. The conformers are also stereochem. characterized, compared with available X-ray structures and with the conformers obtained in our previous MM study using chloro instead of bromo  $\beta$ -pyrrole substituents.  
 IT 131214-86-3  
 RL: PRP (Properties)  
 (conformational anal. of octa- and tetrabromo tetraphenylporphyrins and their Ni(II) and Tb(III) complexes)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2004:1501429 CAPLUS

DOCUMENT NUMBER: 141:287404

TITLE: Physical-chemical properties of tetraphenylporphyrin, its octa-substituents, and complexes with metals in the ground and excited states

AUTHOR(S): Kuznetsova, R. T.; Savenkova, N. S.; Mayer, G. V.

CORPORATE SOURCE: V. D. Kuznetsov Siberian Physical-Technical Institute, Tomsk State University, Tomsk, Russia

SOURCE: Atmospheric and Oceanic Optics (2004), 17(2-3), 149-155

CODEN: AOCOEK ISSN: 1024-8560

PUBLISHER: Institute of Atmospheric Optics

DOCUMENT TYPE: Journal

LANGUAGE: English

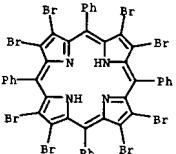
AB The ability of limiting powerful laser radiation (<400 MW/cm<sup>2</sup>) by solns. of tetraphenylporphyrin (TPP) and its derivs., as well as spectral-luminescent and photochem. properties of these mols. at their excitation to different electronic states by radiation of different wavelength and intensity is studied. The quantum yields of fluorescence from Si and Sn excited states and in some cases, the quantum yields and features of phototransformations under exposure to powerful laser radiation were determined.

IT 131214-86-3, 2, 3, 7, 8, 12, 13, 17, 18-Octabromo-5, 10, 15, 20-tetraphenylporphyrin

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process) (phys.-chemical properties of)

RN 131214-86-3 CAPLUS

CN 21H, 23H-Porphine, 2, 3, 7, 8, 12, 13, 17, 18-octabromo-5, 10, 15, 20-tetraphenyl-(9Cl) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2004:1484631 CAPLUS

DOCUMENT NUMBER: 141:184088

TITLE: Polyhalogenated porphyrinic derivatives with indium and thallium: the X-ray structures of ( $\beta$ -C14TPP)Tl(C1) and ( $\beta$ -TpTPP)Tl(C1)

AUTHOR(S): Raptopoulou, Catherine; Daphnomili, Dimitra; Karamalides, Athanassios; Di Vaira, Massimo; Terzis, Aris; Coutsoukos, Athanassios G.

CORPORATE SOURCE: Demokritos, NCRS, Athens, 15310, Greece

SOURCE: Polyhedron (2004), 23(10), 1777-1784

CODEN: PLYHDE ISSN: 0277-5387

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis and spectroscopic characterization of (Porph)M(C1) where H2Porph are TpTPP (tetraphenylporphyrin), TPY (tetra- $\beta$ -chlorotetraphenylporphyrin),  $\beta$ -C14TPP (tetra- $\beta$ -chlorotetraphenylporphyrin),  $\beta$ -C18TPP (octa- $\beta$ -bromotetraphenylporphyrin), and M = In or Tl are reported. UV-visible and NMR spectroscopies of the title complexes confirm the proposed mol. formulas and are described extracting all plausible information. The studyis completed by three x-ray structures of ( $\beta$ -C14TPP)Tl(C1), ( $\beta$ -C14TPP)In(C1) and ( $\beta$ -TpTPP)Tl(C1). Compds. ( $\beta$ -C14TPP)Tl(C1) and ( $\beta$ -C14TPP)In(C1) are isostructural and they were treated in a similar way. The chloride substituents on the porphyrin core are disordered in both compds. and they were refined anisotropically with occupation factors free to vary. The porphyrin core is saddle distorted while there is no twist distortion as judged by the large values of the dihedral angles formed between the Ph rings and the C20N4 mean plane. In ( $\beta$ -TpTPP)Tl(C1), the dihedral angles between the pentafluorophenyl rings and C20N4 are very close to the ideal value of 90°.

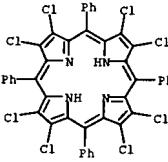
IT 120644-25-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for preparation of indium and thallium porphyrin complexes)

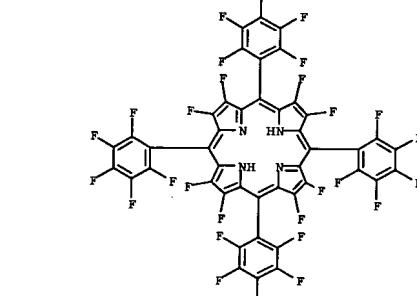
RN 120644-25-9 CAPLUS

CN 21H, 23H-Porphine, 2, 3, 7, 8, 12, 13, 17, 18-octachloro-5, 10, 15, 20-tetraphenyl-(9Cl) (CA INDEX NAME)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PAGE 1-A



PAGE 2-A

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2004:400569 CAPLUS

DOCUMENT NUMBER: 141:133068

TITLE: Electronic Spectroscopy, Photophysical Properties, and Emission Quenching Studies of an Oxidatively Robust Perfluorinated Platinum Porphyrin

AUTHOR(S): Lai, Siu-Wai; Hou, Yuan-Jun; Che, Chi-Ming; Pang, Hei-Leung; Wong, Kwok-Yin; Chang, Chi K.; Zhu, Mianrong

CORPORATE SOURCE: Department of Chemistry and Open Laboratory of Chemical Biology of the Institute of Molecular Technology for Drug Discovery and Synthesis, The University of Hong Kong, Hong Kong, P.R.C. Rep. China

SOURCE: Inorganic Chemistry (2004), 43(12), 3724-3732

CODEN: INOCAJ ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:133068

AB The highly electron-deficient,  $\beta$ -octafluorinated meso-tetrakis(pentafluorophenyl)porphyrin (H2Pt28TPP) was metalated with Pt to afford the oxidatively robust lumiphor [PtF28TPP], and its x-ray structure shows that the porphyrin core exists in a slightly saddle-shaped conformation. The absorption spectrum of [PtF28TPP] in CH2Cl2 displays a near-UV Soret band (B) at 383 nm and two visible Q(1,0) and Q(0,0) bands at 501 and 533 nm, resp. These absorption bands of [PtF28TPP] are blue-shifted from those in [PtF20TPP] (390, 504, and 538 nm, resp.) and [PtTPP] (401, 509, and 539 nm, resp.). Excitation of [PtF28TPP] in CH2Cl2 at the Soret or Q(1,0) or Q(0,0) band gave phosphorescence with peak maximum at 650 nm (lifetime 5.8  $\mu$ s) and a weak shoulder at 712 nm. Both the emission lifetime and quantum yield vary with solvent polarity, and plots of  $\tau$  vs. EK and  $\Phi$  vs. EK (EK is the empirical solvent polarity parameter based on the hypochromic shift of the longest wavelength absorption of the [Mo(CO)4(C5H4N)2Cl:CH2C6H5] complex) with increasing solvent polarity show linear correlation, indicating that the emission is sensitive to the local environment/medium. Electrochemical studies on [PtF28TPP] by cyclic voltammetry showed no porphyrin-centered oxidation at potential  $\sim$  1.5 V vs. Ag/AgNO3, demonstrating that [PtF28TPP] is more resistant toward oxidation than [PtF20TPP] ( $E1/2 = -1.33$  V)and [PtTPP] ( $E1/2 = 0.97$  V). The porphyrin-centered reduction of [PtF28TPP] occurs at  $\sim$  0.75 and  $\sim$  1.18 V, which is anodically shifted from those at  $\sim$  1.06 and  $\sim$  1.55 V in [PtF20TPP], resp. Hence, [PtF28TPP] exhibits superior photostability and quenching of the emission of [PtF28TPP] by O2, alc., catechol, and butylamine reveals that [PtF28TPP] is an oxidatively robust material with medium-sensitive photoluminescence properties.

IT 121399-88-0

RL: RCT (Reactant); RACT (Reactant or reagent) (reactant for preparation of platinum perfluorinated porphyrin complex)

RN 121399-88-0 CAPLUS

CN 21H, 23H-Porphine, 2, 3, 7, 8, 12, 13, 17, 18-octafluoro-5, 10, 15, 20-tetrakis(pentafluorophenyl) (9Cl) (CA INDEX NAME)

16 ANSWER 6 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:356835 CAPLUS  
 DOCUMENT NUMBER: 141:359806  
 TITLE: Highly brominated porphyrins: synthesis, structure and their properties  
 AUTHOR(S): Bhuparpa, Puttaiah; Purushothaman, Bhavana; Vittal, Jagadees J.  
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology-Madras, Chennai, 600 036, India  
 SOURCE: Journal of Porphyrins and Phthalocyanines (2003), 7(9 & 10), 682-692  
 CODEN: JPPHWZ ISSN: 1088-4246  
 PUBLISHER: Society of Porphyrins & Phthalocyanines  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

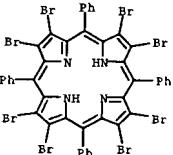
AB This article reports the 1st bromination of  $\beta$ -pyrrole and meso-Ph groups of the 5,10,15,20-tetrakis(3',5'-dimethoxyphenyl)porphinacopper(I) I to generate highly brominated porphyrin, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2',6'-dibromo-3',5'-dimethoxyphenyl)-porphinacopper(II), Cu<sup>2+</sup>(3',5'-DMP)PBr<sub>16</sub> complex. Its crystal structure exhibited unusual five-coordination geometry with saddle-shaped conformation of the porphyrin core. M<sup>2+</sup>(3',5'-DMP)PBr<sub>16</sub> and its metal complexes exhibited large anodic shift of oxidation potentials with marginal changes in reduction potentials relative to their corresponding octabromotetraphenylporphyrin, MTPPBr<sub>8</sub> derivatives. The enhanced electron deficiency of the Zn<sup>2+</sup>(3',5'-DMP)PBr<sub>16</sub> complex was probably by axial ligation of various Lewis bases with differing pKa values. The Zn<sup>2+</sup>(3',5'-DMP)PBr<sub>16</sub> complex exhibited decrease in equilibrium const. for the ligation of bases relative to sterically unhindered ZnTPPBr<sub>8</sub>. This was ascribed to the sterics induced by the bulky ortho-bromo Ph substituents that prevents the facile binding of Lewis bases to the Zn(II)-center.

IT 131214-86-3

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process); (cyclic voltammetry of)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-(9CI) (CA INDEX NAME)



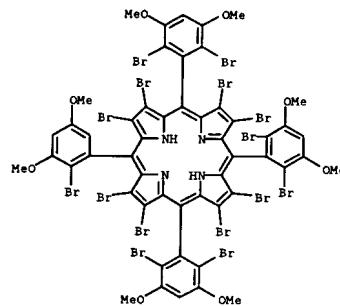
IT 775318-93-9P 775318-94-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 775318-93-9 CAPLUS

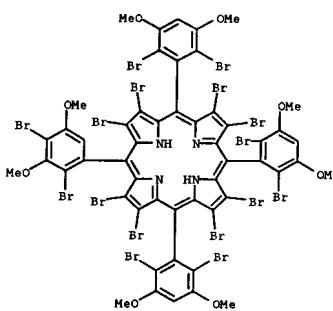
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-(2-bromo-3,5-dimethoxyphenyl)-10,15,20-tris(2,6-dibromo-3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

16 ANSWER 6 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 775318-94-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-(2,4-dibromo-3,5-dimethoxyphenyl)-10,15,20-tris(2,6-dibromo-3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



IT 775318-89-3P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent) (preparation, cyclic voltammetry and reactant for preparation of nickel and zinc highly brominated porphyrin complexes)

16 ANSWER 6 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 ACCESSION NUMBER: 2004:356825 CAPLUS  
 DOCUMENT NUMBER: 141:310404  
 TITLE: Synthesis and electrochemical investigation of covalently linked porphyrin dimers containing a  $\beta$ -brominated subunit. Crystal structure of H<sub>2</sub>(tripp-tpp(Br8))H<sub>2</sub>

AUTHOR(S): Ou, Zhongping; Tagliatesta, Pietro; Senge, Mathias O.; Shao, Jianqiu; Kadish, Karl M.  
 CORPORATE SOURCE: Department of Chemistry, University of Houston, Houston, TX, 77204-5003, USA  
 SOURCE: Journal of Porphyrins and Phthalocyanines (2003), 7(9 & 10), 595-609  
 CODEN: JPPHWZ ISSN: 1088-4246  
 PUBLISHER: Society of Porphyrins & Phthalocyanines  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Ten meso-tetraphenyl-porphyrin-type hetero-dimers containing a partly or completely  $\beta$ -brominated subunit were synthesized and characterized by UV-visible spectroscopy, cyclic voltammetry and spectro-electrochem., showing the presence of low electronic interactions between the two subunits. The investigated compds. are represented as M[tripp-tpp(Br8)]M and M[tripp-tpp(Br8)]M (M = Zn, Ni, Co and Cu) where tripp-tpp(Br4) is the tetra-anion of 1-[5-(10,15,20-triphenyl-porphyrinyl)]-4-[10-(2,3,12,13-tetra-bromo-porphyrinyl)]-benzene and tripp-tpp(Br8) is the tetra-anion of 1-[5-(10,15,20-triphenyl-porphyrinyl)]-4-[10-(2,3,7,8,12,13,17,18-octabromo-porphyrinyl)]-benzene. One of the synthesized dimers, H<sub>2</sub>(tripp-tpp(Br8))H<sub>2</sub>, was characterized by a single-crystal X-ray investigation.

IT 552887-02-2P

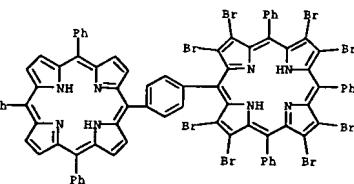
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis, crystal structure, cyclic voltammetry, and electrochem. investigation of covalently linked porphyrin dimers containing a  $\beta$ -brominated subunit)

RN 552887-02-2 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15-triphenyl-20-(4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 111 THERE ARE 111 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

16 ANSWER 7 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:356825 CAPLUS  
 DOCUMENT NUMBER: 141:310404  
 TITLE: Synthesis and electrochemical investigation of covalently linked porphyrin dimers containing a  $\beta$ -brominated subunit. Crystal structure of H<sub>2</sub>(tripp-tpp(Br8))H<sub>2</sub>

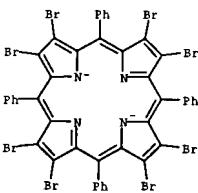


REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:354172 CAPLUS  
 DOCUMENT NUMBER: 141:106158  
 TITLE: Theoretical AM1 study of acidity of porphyrins, azaporphyrins and porphyrazines  
 AUTHOR(S): Stushin, Pavel A.  
 CORPORATE SOURCE: Department of Organic Chemistry, Ivanovo State University of Chemical Technology, Ivanovo, 153460, Russia  
 SOURCE: Journal of Porphyrins and Phthalocyanines (2003), 7(11 & 12), 813-832  
 PUBLISHER: Society of Porphyrins & Phthalocyanines  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The structure-acidity relationship in the series of non-substituted, meso- or  $\beta$ -substituted and  $\beta,\beta$ -annulated porphyrins and porphyrazines have been studied using the AM1 method with UHF basis set. With this purpose, heats of formation have been determined for the geometry optimized structures of the free base macrocycles and corresponding monoanions and dianions formed by deprotonation. Calculated first deprotonation enthalpy values show correlation with available exptl.  $pK_a$  values and can be used for prediction of acidity. For porphyrazines bearing electron-withdrawing substituents or  $\pi$ -deficient annulated heteroarenes the dianions have lower heats of formation than the corresponding neutral species and such porphyrazines are easily deprotonated upon dissoln. in basic solvents (pyridine, DMF). For porphyrazines with annulated 5-member heteroarenes it is predicted that deprotonation of peripheral NH groups should occur more easily than deprotonation of the internal NH groups. The influence of different types of annulation of 5- and 6-membered heteroarenes to the porphyrazine core on the stability of the macrocyclic system and its acidity are also discussed.

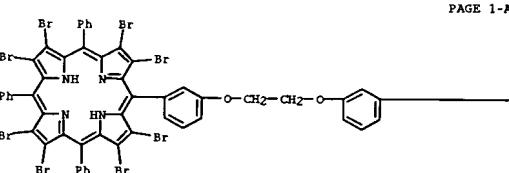
IT 717911-35-8  
 RL: PRP (Properties)  
 (dianion, formation enthalpy; theor. AM1 structure-acidity study of porphyrins, azaporphyrins and porphyrazines)  
 RN 717911-35-8 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, ion(2-) (9CI) (CA INDEX NAME)



IT 131214-86-3  
 RL: PRP (Properties)  
 (formation enthalpy and deprotonation enthalpy; theor. AM1 structure-acidity study of porphyrins, azaporphyrins and porphyrazines)

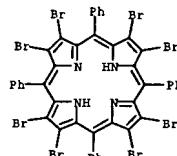
L6 ANSWER 9 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:377463 CAPLUS  
 DOCUMENT NUMBER: 141:342314  
 TITLE: Covalently linked bisporphyrins bearing tetraphenylporphyrin and perbromoporphyrin units: synthesis and their properties  
 AUTHOR(S): Bhayappa, Futtahal; Krishnan, V.  
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Madras, Chennai, 600 036, India  
 SOURCE: Journal of Chemical Sciences (Bangalore, India) (2004), 116(2), 71-78  
 PUBLISHER: Indian Academy of Sciences  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A series of covalently linked bisporphyrins bearing meso-tetraphenylporphyrin (TPP) and octabromotetraphenylporphyrin (OBTPP) units have been synthesized and characterized. Electrochem. studies on these bisporphyrins showed an anodic shift (apprx. 30-60 mV) of the TPP unit and a cathodic shift (apprx. 40-80 mV) of OBTPP in redox potentials. Further, steady-state fluorescence studies on bisporphyrins indicated dramatic decrease in fluorescence quantum yields of the TPP moiety. Electrochem. redox and fluorescence data seem to suggest the possible existence of intramol. interactions in these bisporphyrins.

IT 770714-96-0  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (synthesis, electrochem. redox, and fluorescence properties of covalently linked bisporphyrins and their metal complexes bearing tetraphenylporphyrin and perbromoporphyrin)  
 RN 770714-96-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15-triphenyl-20-[3-[2-[3-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenoxy]ethoxy]phenyl]- (9CI) (CA INDEX NAME)

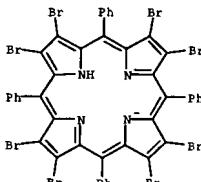


PAGE 1-A

L6 ANSWER 8 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, ion(1-) (9CI) (CA INDEX NAME)



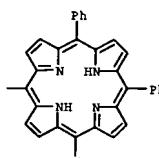
IT 717911-25-6  
 RL: PRP (Properties)  
 (monoanion, formation enthalpy; theor. AM1 structure-acidity study of porphyrins, azaporphyrins and porphyrazines)  
 RN 717911-25-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, ion(1-) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

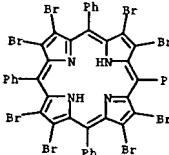
L6 ANSWER 9 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B

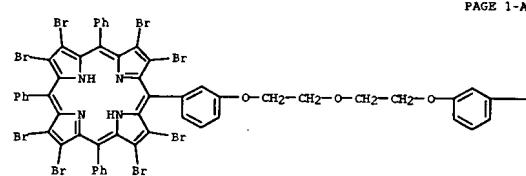


IT 131214-86-3P 770715-01-0P  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
 (synthesis, electrochem. redox, and fluorescence properties of covalently linked bisporphyrins and their metal complexes bearing tetraphenylporphyrin and perbromoporphyrin)

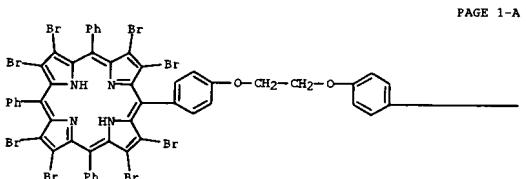
RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, ion(1-) (9CI) (CA INDEX NAME)



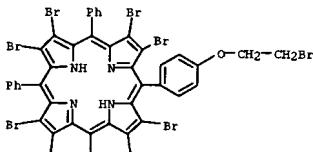
RN 770715-01-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15-triphenyl-20-[3-[2-[3-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenoxy]ethoxy]phenyl]- (9CI) (CA INDEX NAME)



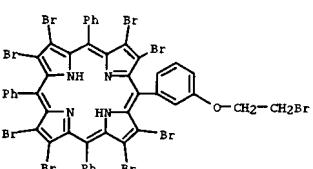
IT 770714-95-9P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); PACT (Reactant or reagent)  
 (synthesis, electrochem, redox, and fluorescence properties of covalently linked bisporphyrins and their metal complexes bearing tetraphenylporphyrin and perbromoporphyrin)  
 RN 770714-95-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15-triphenyl-20-[4-[2-(4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenoxy]ethoxy]phenyl]- (9CI) (CA INDEX NAME)



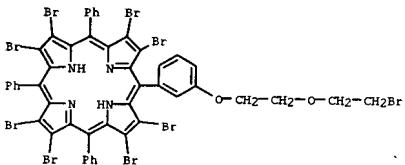
IT 213414-00-7P 770714-93-7P 770714-94-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis, electrochem, redox, and fluorescence properties of covalently linked bisporphyrins and their metal complexes bearing tetraphenylporphyrin and perbromoporphyrin)  
 RN 213414-00-7 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-[4-(2-bromoethoxy)phenyl]-10,15,20-triphenyl- (9CI) (CA INDEX NAME)



IT 770714-93-7 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-[3-(2-bromoethoxy)phenyl]-10,15,20-triphenyl- (9CI) (CA INDEX NAME)



RN 770714-94-8 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-[3-(2-bromoethoxy)ethoxy]phenyl]-10,15,20-triphenyl- (9CI) (CA INDEX NAME)



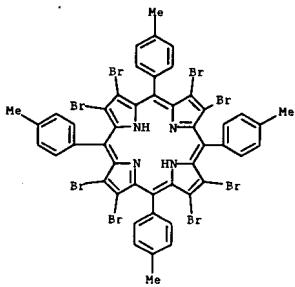
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AUTHOR(S): George, Regimol G.; Padmanabhan, M.  
 SCHOOL OF CHEMICAL SCIENCES, MAHATMA GANDHI UNIVERSITY, KOTTAYAM, 696 560, INDIA  
 SOURCE: PROCEEDINGS - INDIAN ACADEMY OF SCIENCES, CHEMICAL SCIENCES (2003), 115(4), 263-271  
 CODEN: PIADM; ISSN: 0253-4134

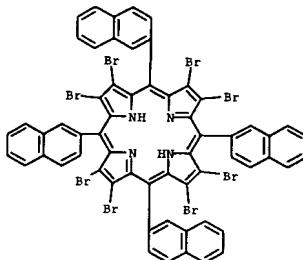
PUBLISHER: Indian Academy of Sciences  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A series of porphyrins with tolyl and naphthyl substituents at the meso positions, their octabromo derivs. (OBPs) with Br substituents at  $\beta$ -pyrrole positions are synthesized and characterized by chemical anal.,  $^1$ H NMR and electronic spectral studies. It is seen that all the OBPs exhibit pronounced red shifts in both the Soret and Q bands of their electronic spectra compared to their non-brominated form in various polar and nonpolar solvents, the energy difference  $\Delta_{\text{hvin.v}}$  being in the range 2300-2700 cm<sup>-1</sup>. The high energy B band of naphthyl porphyrins (both brominated and nonbrominated) are found to be more red-shifted than that of tolyl porphyrins, owing to the noticeable mesomeric effect of the naphthyl groups. Detailed spectral studies reveal that while none of the nonbrominated porphyrin show solvent-dependent change in their B and Q bands, all the OBPs manifest significant shifts depending on the nature of solvents. Solvent-solute interaction can be considered to be of strong dipole-dipole nature for OBPs with polar solvents and of  $\pi$ - $\pi$  type with aromatic non-polar solvents. In the brominated form we find two categories of porphyrins exhibiting distinctly different absorption phenomena in aromatic solvents. The OBPs having meso-groups not shielding the porphyrin  $\pi$ -framework exhibit addnl. absorption peaks (split Soret peaks and broadened Q bands) in some aromatic solvents. This could be explained in terms of  $\pi$ - $\pi$  type donor-acceptor (DA) complex formation between such bromoporphyrins (acceptor) and the aromatic solvent mols. (donor) that is not possible for OBPs that have bulky meso groups that block the approach of aromatic solvent mols. close to the porphyrin framework.

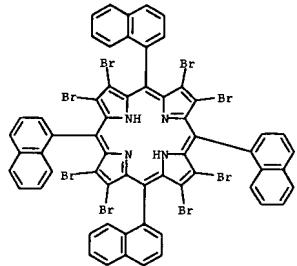
IT 182423-35-4 640730-26-3 640730-27-4  
 640730-28-5 640730-29-6  
 RL: PRP (Properties)  
 (solvent effects on absorption spectra of meso-aryl substituted octabromoporphyrins)  
 RN 182423-35-4 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-methylphenyl)- (9CI) (CA INDEX NAME)



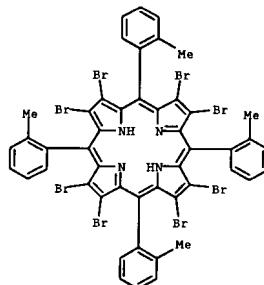
RN 640730-26-3 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetra-1-naphthalenyl- (9CI) (CA INDEX NAME)



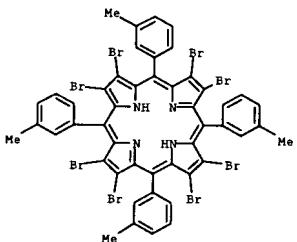
RN 640730-28-5 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2-methylphenyl)- (9CI) (CA INDEX NAME)



RN 640730-27-4 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetra-2-naphthalenyl- (9CI) (CA INDEX NAME)



RN 640730-29-6 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(3-methylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2003:762928 CAPLUS

DOCUMENT NUMBER: 140:103814

TITLE: Studies on some new meso-aryl substituted

octabromo-porphyrins and their Zn(II) derivatives

AUTHOR(S): George, Regimol G. I. Padmanabhan, M.

CORPORATE SOURCE: School of Chemical Sciences, Mahatma Gandhi

UNIVERSITY, Kottayam, 686560, India

SOURCE: Polyhedron (2003), 22(23), 3145-3154

CODEN: PLYHDE; ISSN: 0277-5387

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Porphyrins with various tolyl (H2TTP) and naphthyl substituents (H2TNHP) at the meso-positions, their octabromo derivs. (H2TTPB and H2TNPB) with Br substituents at  $\beta$ -pyrrole positions and also their Zn(II) derivs. were synthesized and characterized by 1H NMR, electronic, fluorescence and electrochem. studies. These have the meso-carbons bonded to tolyl moieties at ortho-, meta- and para-positions of the tolyl groups and at the  $\alpha$ - or  $\beta$ -position of the naphthyl group. For the octabromoporphyrins, pronounced deshielding of NH protons and a moderate shift of meso-aryl protons to a lower  $\delta$  value are observed compared to their nonbrominated species. The electronic spectra of ZnTTP and ZnTNHP have almost the same B and Q bands while the B band of their free-base analogs have H2TNHP absorbing at a higher wavelength than H2TTP. All the octabromo derivs. exhibit a pronounced red shift for both B and Q bands (compared to their nonbrominated forms) and show meso-substituent dependent change in both free-base and metalated forms. The above observations are interpreted in terms of moderate conjugative interaction of the aryl substituent with the  $\pi$  framework and also in terms of energy level reordering which alters the HOMO-LUMO gap. Consistent with the absorption spectral data the emission bands of all the bromoporphyrins also are red shifted considerably. Significant decrement in quantum yield ( $\Phi$ ) was observed for the bromo compds. While the  $\Phi$  of nonbrominated porphyrins is higher than their Zn(II) derivs. the reverse order is observed for the bromo derivs. The ability of the Zn<sup>2+</sup> ion to make the bromoporphyrins resistant to distortion by bridging the central cavity can be attributed as the cause for this interesting observation. Cyclic voltammetric studies exhibit characteristic quasi-reversible/irreversible oxidation-reduction features for all the free-bases and Zn(II) derivs. The bromo derivs. however, manifest marginally harder oxidation and very easy reduction

features. The data are interpreted in terms of electron withdrawing ability of Br atoms and to reordering of HOMO and LUMO levels due to distortion in the porphyrin ring.

IT 182423-35-4P 640730-26-3P 640730-27-4P

640730-28-5P 640730-29-6P

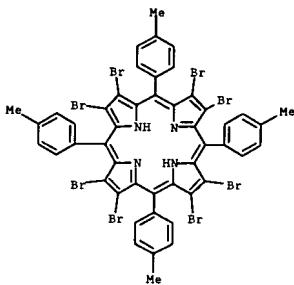
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation, electrochem. properties, metalation with zinc and electronic

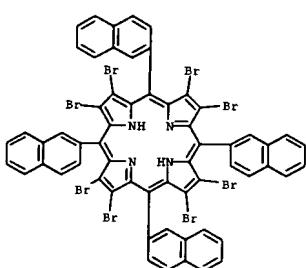
and fluorescence spectra of meso-tetraaryl substituted octabromoporphyrin)

RN 182423-35-4 CAPLUS

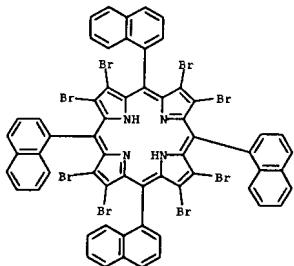
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-methylphenyl)- (9CI) (CA INDEX NAME)



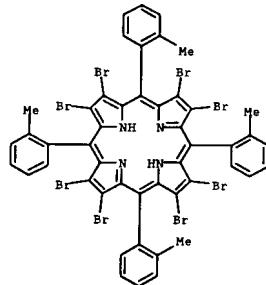
RN 640730-26-3 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetra-1-naphthalenyl- (9CI) (CA INDEX NAME)



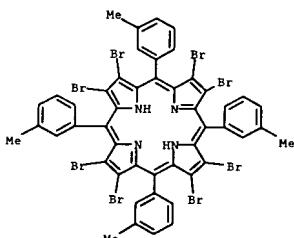
RN 640730-28-5 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2-methylphenyl)- (9CI) (CA INDEX NAME)



RN 640730-27-4 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetra-2-naphthalenyl- (9CI) (CA INDEX NAME)

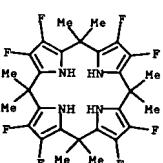


RN 640730-29-6 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(3-methylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2003:623230 CAPLUS  
DOCUMENT NUMBER: 139:370552  
TITLE: Fluorinated calixpyrroles: anion-binding extractants that reduce the Hofmeister bias  
AUTHOR(S): Levitskaya, Tatiana G.; Marquez, Manuel; Sessler, Jonathan L.; Shriner, James A.; Vercouter, Thomas; Moyer, Bruce A.  
CORPORATE SOURCE: Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37830-6119, USA  
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (17), 2248-2249  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB  $\beta$ -Octafluoro-meso-octamethylcalix[4]pyrrole (I) and  $\beta$ -decafluoro-meso-decamethylcalix[5]pyrrole (II) were found to extract cesium salts of smaller anions (bromide and chloride for I and nitrate for II) as effectively as that of iodide into nitrobenzene (NB) thereby overcoming the Hofmeister bias normally observed for processes of this type.  
IT 311804-81-6  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)  
(cesium salt solvent extn with fluorinated calixpyrroles and attenuation of Hofmeister series)  
RN 311804-81-6 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2003:1563277 CAPLUS

DOCUMENT NUMBER: 139:239081

TITLE: Synthesis and Structural Characterization of

Porphyrinic Enediynes: Geometric and Electronic

Effects on Thermal and Photochemical Reactivity

Chandra, Tilak; Kraft, Brian J.; Huffman, John C.,

Zaleski, Jeffrey M.

COPORATE SOURCE: Department of Chemistry and Molecular Structure

Center, Indiana University, Bloomington, IN,

47405-7102, USA

SOURCE: Inorganic Chemistry (2003), 42(17), 5158-5172

PUBLISHER: CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: American Chemical Society

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:239081

AB The authors report the preparation of 5,10,15,20-tetr phenyl-2,3,7,8,12,13,17,18-octakis(phenylethynyl)porphine and its Ni(II), Zn(II), Mg(II), and Cu(II) complexes, as well as select trimethylsilyl ethynyl derivs. The x-ray structures of the octakis(phenylethynyl) compds. show systematic deviations from planarity (Ni(II), 0.2851 Å; Zn(II), 0.0304 Å) as a function of the central cation. These geometric distortions are reflected in bathochromic shifts of the Soret and Q bands (Ni(II), 497, 604, and 650 nm; Mg(II), 515, 595, 642, and 705 nm) which loosely correlate with increasing planarity of the structure. Similarly, vibrational modes involving the octa-substituted porphyrin core exhibit shifts to lower frequency as a function of increasing planarity in the solution-state resonance Raman spectra ( $\lambda_{exc} = 501.7$  nm) of these compds. Analogous trends are also observed in their solid-state electronic and resonance Raman spectra, indicating that the structural distortions within the octakis(phenylethynyl) series are preserved in solution. Comparison of the saddle distortion of the octa-substituted Ni(II) compound with the ruffle/saddle distortions of the pentakis and hexakis Ni(II) derivs. reveals some influence of asym. peripheral substitution on geometric structure. These Ni(II) derivs. also exhibit systematic red shifts in their electronic spectra as a function of the number of conjugated alkyne units (apprx.13 nm/alkyne), revealing participation of the enediyne units in the electronic ground and excited states. The solid-state Bergman cyclization temps. of the phenylethynyl compds. vary markedly as a function of planarity, and correlate loosely with alkyne termini separation (Ni(PA)8, 4.00 Å, 281°; MgP(PA)8, 3.77 Å, 244°). In solution, both thermal and photochem. activation of the free-base octakis(phenylethynyl) compound lead to formal reduction of the porphyrin backbone via H-atom addition at opposing meso-positions. Generation of a common product suggests that both thermal and photochem. pathways to Bergman cyclization in solution contain significant activation barriers to formation of the 1,4-Ph diradical intermediate, and under these solution conditions, alternate reaction channels are more thermodynamically favorable.

IT 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-

-tetraphenylporphine

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of ethynyl-substituted tetraphenylporphines and their magnesium and transition metal complexes)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetr phenyl-

(9CI) (CA INDEX NAME)

139:239081 CAPLUS

DOCUMENT NUMBER: 139:239081

TITLE: Synthesis and Structural Characterization of

Porphyrinic Enediynes: Geometric and Electronic

Effects on Thermal and Photochemical Reactivity

Chandra, Tilak; Kraft, Brian J.; Huffman, John C.,

Zaleski, Jeffrey M.

COPORATE SOURCE: Department of Chemistry and Molecular Structure

Center, Indiana University, Bloomington, IN,

47405-7102, USA

SOURCE: Inorganic Chemistry (2003), 42(17), 5158-5172

PUBLISHER: CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: American Chemical Society

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:239081

AB The authors report the preparation of 5,10,15,20-tetr phenyl-2,3,7,8,12,13,17,18-octakis(phenylethynyl)porphine and its Ni(II), Zn(II), Mg(II), and Cu(II) complexes, as well as select trimethylsilyl ethynyl derivs. The x-ray structures of the octakis(phenylethynyl) compds. show systematic deviations from planarity (Ni(II), 0.2851 Å; Zn(II), 0.0304 Å) as a function of the central cation. These geometric distortions are reflected in bathochromic shifts of the Soret and Q bands (Ni(II), 497, 604, and 650 nm; Mg(II), 515, 595, 642, and 705 nm) which loosely correlate with increasing planarity of the structure. Similarly, vibrational modes involving the octa-substituted porphyrin core exhibit shifts to lower frequency as a function of increasing planarity in the solution-state resonance Raman spectra ( $\lambda_{exc} = 501.7$  nm) of these compds. Analogous trends are also observed in their solid-state electronic and resonance Raman spectra, indicating that the structural distortions within the octakis(phenylethynyl) series are preserved in solution. Comparison of the saddle distortion of the octa-substituted Ni(II) compound with the ruffle/saddle distortions of the pentakis and hexakis Ni(II) derivs. reveals some influence of asym. peripheral substitution on geometric structure. These Ni(II) derivs. also exhibit systematic red shifts in their electronic spectra as a function of the number of conjugated alkyne units (apprx.13 nm/alkyne), revealing participation of the enediyne units in the electronic ground and excited states. The solid-state Bergman cyclization temps. of the phenylethynyl compds. vary markedly as a function of planarity, and correlate loosely with alkyne termini separation (Ni(PA)8, 4.00 Å, 281°; MgP(PA)8, 3.77 Å, 244°). In solution, both thermal and photochem. activation of the free-base octakis(phenylethynyl) compound lead to formal reduction of the porphyrin backbone via H-atom addition at opposing meso-positions. Generation of a common product suggests that both thermal and photochem. pathways to Bergman cyclization in solution contain significant activation barriers to formation of the 1,4-Ph diradical intermediate, and under these solution conditions, alternate reaction channels are more thermodynamically favorable.

IT 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-

-tetraphenylporphine

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of ethynyl-substituted tetraphenylporphines and their magnesium and transition metal complexes)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetr phenyl-

(9CI) (CA INDEX NAME)

ACCESSION NUMBER: 2003:414405 CAPLUS

DOCUMENT NUMBER: 138:409450

TITLE: Optical recording media having super resolution mask

layer and method for recording/reading thereof

INVENTOR(S): Sato, Tsutomu; Tomura, Tatsuya; Ueno, Yasunobu;

PATENT ASSIGNEE(S): Ricoh Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

IT 139944-26-6

RL: TEM (Technical or engineered material use); USES (Uses)

(super resolution mask layer in optical recording media)

RN 139944-26-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-

-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 2-A

F

139944-26-6

RL: TEM (Technical or engineered material use); USES (Uses)

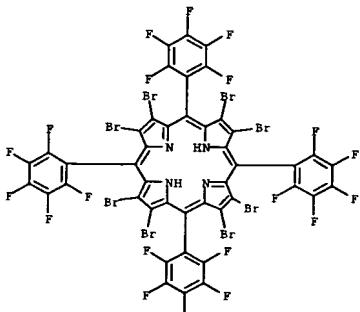
(super resolution mask layer in optical recording media)

RN 139944-26-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-

-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



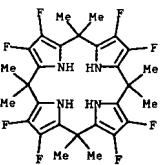
L6 ANSWER 15 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:385522 CAPLUS  
 DOCUMENT NUMBER: 139:100832  
 TITLE: Single Side Strapping: A New Approach to Fine Tuning the Anion Recognition Properties of Calix[4]pyrroles  
 AUTHOR(S): Lee, Chang-Hee; Na, Hee-Kyung; Yoon, Dae-Wi; Won, Dong-Hoon; Cho, Won-Seob; Lynch, Vincent M.; Shevchuk, Sergey V.; Sessler, Jonathan L.  
 CORPORATE SOURCE: Department of Chemistry, Kangwon National University, Chun-Chon, 200-701, S. Korea  
 SOURCE: Journal of the American Chemical Society (2003), 125 (24), 7301-7306  
 CODEN: JACSAU; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:100832

AB Three calix[4]pyrroles bearing m-cresol-derived diether straps of different lengths on one side of the tetrapyrrolic core were synthesized and characterized. Structural information for an analogous diester bridged strapped system reported previously (Yoon, D. W.; Hwang, H.; Lee, C. H. Angew. Chem. Int. Ed. Engl. 2002, 41, 1757-1759) is also provided as are bromide and chloride anion affinities for all four systems determined by

Isothermal Titration Calorimetry (ITC) in acetonitrile. Although both sets of the strapped calix[4]pyrroles displayed enhanced affinities for chloride and bromide anion, differences were seen among the various receptors that support the conclusion that the anion binding ability of calixpyrrole-type systems can be effectively tuned by modifying the length and nature of the bridging straps. In the specific case of the diether systems, the largest chloride affinity was seen with the shortest strap, whereas the largest affinity for bromide anion was recorded in the case of the longest strap. As well as supporting <sup>1</sup>H NMR spectroscopic studies, it is postulated that not only cavity size per se, but also the ability of the aryl portion of the strap to serve as a C-H bond donor site are important in regulating the observed anion affinities.

IT 311804-81-6  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PYF (Physical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); (complexation of halide salts; single side strapping approach to fine tuning anion recognition properties of calix[4]pyrroles)

RN 311804-81-6 CAPLUS  
 CN 21H, 23H-Porphine, 2, 3, 7, 8, 12, 13, 17, 18-octafluoro-5, 10, 15, 20, 22, 24-hexahydro-5, 5, 10, 10, 15, 15, 20, 20-octamethyl- (9CI) (CA INDEX NAME)



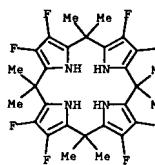
IT 311804-88-3 560094-16-8 560094-21-5

L6 ANSWER 15 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYF (Physical process); FORM (Formation, nonpreparative); PROC (Process); (single side strapping approach to fine tuning anion recognition properties of calix[4]pyrroles)

RN 311804-88-3 CAPLUS  
 CN 1-Butanaminium, N,N,N-triethyl-, chloride, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

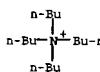
CH 1

CRN 311804-81-6  
 CMF C28 H28 F8 N4



CH 2

CRN 1112-67-0  
 CMF C16 H36 N . Cl



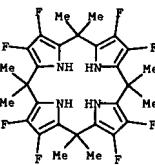
● Cl<sup>-</sup>

RN 560094-16-8 CAPLUS  
 CN Potassium(1+), (4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane-  
 xN1,xN10,xO4,xO7,xO13,xO16,xO21,  
 xO24)-, chloride, compd. with 2,3,7,8,12,13,17,18-octafluoro-  
 5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-  
 porphine (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 311804-81-6  
 CMF C28 H28 F8 N4

L6 ANSWER 15 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CH 2

CRN 1643-19-2  
 CMF C16 H36 N . Br



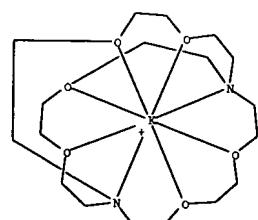
● Br<sup>-</sup>

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RN 560094-21-5 CAPLUS  
 CN 1-Butanaminium, N,N,N-triethyl-, bromide, compd. with 2,3,7,8,12,13,17,18-  
 octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-  
 21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 311804-81-6  
 CMF C28 H28 F8 N4



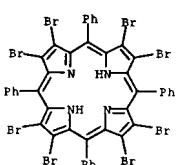
● Cl<sup>-</sup>

L6 ANSWER 16 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:290712 CAPLUS  
 DOCUMENT NUMBER: 139:45848  
 TITLE: Differential substituent effects of  $\beta$ -halogens in water-soluble porphyrins  
 AUTHOR(S): Biffinger, Justin C.; Sun, Haoran; Nelson, Andrew P.; DiMaggio, Stephen G.  
 CORPORATE SOURCE: Department of Chemistry, University of Nebraska, Lincoln, NE, USA  
 SOURCE: Organic & Biomolecular Chemistry (2003), 1(4), 733-736  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:45848

AB The 1st water-soluble  $\beta$ -octafluorinated porphyrins, 5,10,15,20-tetrakis(4-sulfonatophenyl)-2,3,7,8,12,13,17,18-octafluoroporphyrin, 1, 2,3,7,8,12,13,17,18-octafluoroporphyrin, 2, were prepared and their aqueous aggregation, acid-base, and optical properties were characterized. The porphyrins are tetraanionic at neutral pH (at pH = 3-11 for 1 and pH = 0-9 for 2). Semiempirical (AM1) calcns. provide evidence that somewhat unusual acidity characteristics of the fluorinated compds. (with respect to similar brominated porphyrins) can be rationalized solely from chemical hardness and electronegativity arguments. The large conformational differences seen in the structures of brominated and fluorinated water-soluble porphyrins have little impact upon N-H acidity. Metalation of 1 and 2 with ZnCl<sub>2</sub> yielded the corresponding Zn complexes, which were characterized by optical spectroscopy and electrochem.

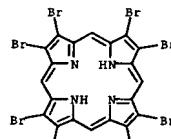
IT 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin 144811-83-6, 2,3,7,8,12,13,17,18-Octabromoporphyrin 541528-61-4

RL: PRP (Properties)  
 (energy of gas phase acidities from semiempirical AM1 calcns.)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

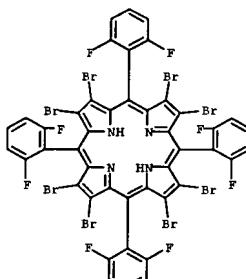


RN 144811-83-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)

L6 ANSWER 16 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

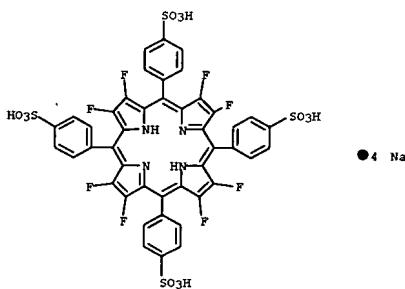


RN 541528-61-4 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-difluorophenyl)- (9CI) (CA INDEX NAME)



IT 541528-56-7P 541528-57-8P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and complexation with zinc and acidity)  
 RN 541528-56-7 CAPLUS  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octafluoro-21H,23H-porphine-5,10,15,20-tetrayl)tetrasodium salt (9CI) (CA INDEX NAME)

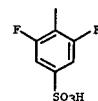
L6 ANSWER 16 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 541528-57-8 CAPLUS  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octafluoro-21H,23H-porphine-5,10,15,20-tetrayl)tetrasodium salt (9CI) (CA INDEX NAME)

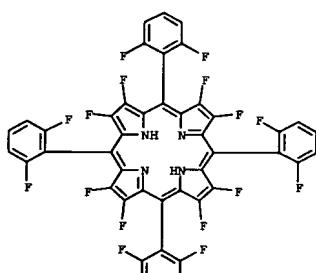
L6 ANSWER 16 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A



● 4 Na

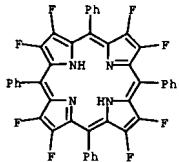
IT 541528-60-3P  
 RL: RCT (Reactant), SPN (Synthetic preparation), PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reactant for preparation of tetrakis(difluorosulphonatophenyl)octafluoroporphyrin)  
 RN 541528-60-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)



PAGE 1-A

IT 186885-28-9, 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetraphenylporphyrin  
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
 (reactant for preparation of tetrakis(sulfonatophenyl)octafluoroporphyrin and energy of gas phase acidities from semiempirical AM1 calcns.)

IT 186885-28-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

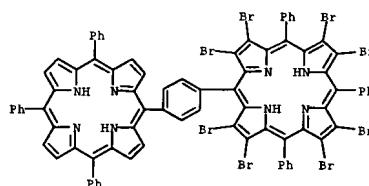


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 17 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:243699 CAPLUS  
 DOCUMENT NUMBER: 139:92612  
 TITLE: Perhalogenated porphyrins as a sink of excitation energy in porphyrin heterodimers  
 AUTHOR(S): Venanzi, Mariano; Tagliatesta, Pietro; Pastorini, Alessandra; Mari, Patrizia; Elisei, Fausto; Latterini, Loreddana; Kadish, Karl M.  
 CORPORATE SOURCE: Dipartimento di Scienze e Tecnologie Chimiche, Univ. Roma-Tor Vergata, Rome, 00133, Italy  
 SOURCE: Journal of Porphyrins and Phthalocyanines (2002), 6(9 & 10), 643-652  
 PUBLISHER: Society of Porphyrins & Phthalocyanines  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The photophysics of a new family of free-base and zinc derivs. of meso-tetraphenylporphyrin heterodimers have been studied by UV-vis absorption, fluorescence and nanosecond flash photolysis techniques. An almost complete (~99%) and directionally controlled transfer of excitation energy from a donor porphyrin moiety was obtained by multiple bromination (four and eight Br substituents in the two series of compds. investigated) on the  $\beta$ -pyrrole positions of the acceptor porphyrin mol. The covalently linked porphyrin dimers populate almost exclusively low energy triplet states because of the extremely efficient intramol. singlet-to-triplet inter system crossing (ISC) process which is enhanced by the multiple heavy atoms substitutions. The nature of the electronic interactions determining the actual relaxation pathway followed by the porphyrin donor-acceptor pair is discussed.

IT 552887-02-2  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
 (perhalogenated porphyrins as sink of excitation energy in porphyrin heterodimers)  
 RN 552887-02-2 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15-triphenyl-20-[4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenyl]- (9CI) (CA INDEX NAME)



IT 131214-86-3, 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo, 5,10,15,20-Tetraphenyl  
 RL: PRP (Properties)  
 (perhalogenated porphyrins as sink of excitation energy in porphyrin heterodimers)  
 RN 131214-86-3 CAPLUS

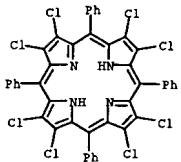
L6 ANSWER 17 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 18 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:226965 CAPLUS  
 DOCUMENT NUMBER: 138:401523  
 TITLE: Electronic Absorption and Resonance Raman Signatures of Hyperporphyrins and Nonplanar Porphyrins  
 AUTHOR(S): Wasbotten, Ingar H.; Conradie, Jeanet; Ghosh, Abhik  
 CORPORATE SOURCE: Institute of Chemistry, Faculty of Science, University of Tromsø, Tromsø, N-9037, Norway  
 SOURCE: Journal of Physical Chemistry B (2003), 107(v 15), 3613-3623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

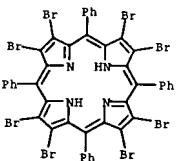
AB We have carried out a broad survey of tetraphenylporphyrin derivs. in relation to their possible hyperporphyrin character. The majority of the free-base tetraphenylporphyrins studied, i.e., TArPH2: Ar = p-X-C6H4, where X = CH3, H, F, CF3, and NO2, when dissolved in trifluoroacetic acid (i.e. when centrally diprotonated), exhibit red-shifted "hyperporphyrin" spectra. The "hyper" features are attributable to phenyl-to-porphyrin charge-transfer transitions. However, certain free-base tetraphenylporphyrins with extremely electron-deficient Ph groups, such as TPFPPh2, do not exhibit hyperporphyrin spectra in trifluoroacetic acid solution. Certain anionic tetraphenylporphyrin derivs. such as T(p-OH-P)Ph2 or Ni[T(p-OH-P)P] dissolved in methanolic Bu4NOH also qualify as hyperporphyrins. The hyper transitions in these cases involve charge transfer from anionic phenolate substituents to the neutral porphyrin core. This study also presents a first systematic resonance Raman spectroscopic exploration of hyperporphyrins. Comparison of the Soret-resonant Raman spectra of various normal, hyper-, and hypo-tetraphenylporphyrin derivs. indicates that the former two categories generally exhibit a more intense v1 band, which is the fully sym. Cmso-Cohenyl stretching vibration, relative to hypoporphyrins such as square-planar nickel tetraarylporphyrins. We have also reinvestigated recent reports of large red shifts observed for the electronic spectra of saddled porphyrins in polar solvents, an effect attributed to increased N-H...solvent hydrogen bonding in polar solvents. Interestingly, we find that such solvent-induced red shifts are observed for the relatively electron-deficient porphyrin BrTPPh2, Cl8TPPh2, and OETTPH2 but not for the relatively electron-rich OETTPH2. Resonance Raman spectra of these saddled porphyrins in different solvents reveal little shift in the high-frequency marker bands, which is consistent with little change in macrocycle conformation with solvent polarity. The observed solvent-induced red shifts in the electronic spectra therefore appear to reflect a largely electronic (as opposed to conformational) effect of N-H...solvent hydrogen bonding in polar solvents. Finally, we also present a chronol. summary of the controversial question as to whether nonplanar deformations are actually responsible for the red-shifted electronic spectra of the majority of nonplanar porphyrins.

IT 120644-25-9,  $\beta$ -Octachloro-meso-tetraphenylporphyrin  
 131214-86-3,  $\beta$ -Octabromo-meso-tetraphenylporphyrin  
 RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process)  
 (electronic absorption and resonance Raman signatures of hyperporphyrins and nonplanar porphyrins)

RN 120644-25-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-(9Cl) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

TITLE: Unusual Aryl-Porphyrin Rotational Barriers in Peripherally Crowded Porphyrins  
 AUTHOR(S): Medforth, Craig J.; Haddad, Raid E.; Muzzi, Cinzia M.; Dooley, Neal R.; Jaquinod, Laurent; Shyr, David C.; Nurco, Daniel J.; Olmstead, Marilyn M.; Smith, Kevin M.; Ma, Jian-Guo; Shelutt, John A.

CORPORATE SOURCE: Department of Chemistry, University of California, Davis, CA, 95616, USA

SOURCE: Inorganic Chemistry (2003), 42(7), 2227-2241

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:347950

AB Previous studies of 5,10,15,20-tetraarylporphyrins showed that the barrier for meso aryl-porphyrin rotation (ΔG,dbldag,ROT) varies as a function of the core substituent M and is lower for a small metal (M = Ni) compared to a large metal (M = Zn) and for a dication (M = 4H2+) vs. a free base porphyrin (M = 2H). This was attributed to changes in the nonplanar distortion of the porphyrin ring and the deformability of the macrocycle caused by the core substituent. X-ray crystallog., mol. mechanics (MM) calcs., and variable temperature (VT) 1H NMR spectroscopy

were used to examine the relation between the aryl-porphyrin rotational barrier and the core substituent M in some novel 2,3,5,7,8,10,12,13,15,17,18,20-dodecarylporphyrins (DARPs), and specifically in some 5,10,15,20-tetraaryl-2,3,7,8,12,13,17,18-octaphenylporphyrins (TAROPPs), where steric crowding of the peripheral groups always results in a very nonplanar macrocycle. X-ray structures of DARPs indicate differences in the nonplanar conformation of the macrocycle as a function of M, with saddle conformations being observed for M = Zn, 2H or M = 4H2+ and saddle and/or ruffle conformations for M = Ni. Variable-temperature NMR studies

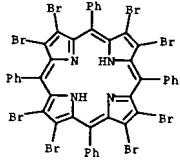
show that the effect of protonation in the TAROPPs is to increase ΔG,dbldag,ROT, which is the opposite of the effect seen for the TARPs, and MM calcs. also predict a strikingly high barrier for the TAROPPs when M = 4H2+. These and other findings suggest that the aryl-porphyrin rotational barriers in the DARPs are closely linked to the deformability of the macrocycle along a nonplanar distortion mode which moves the substituent being rotated out of the porphyrin plane.

IT 131214-86-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (Suzuki coupling reaction with phenylboronic acids)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-(9Cl) (CA INDEX NAME)



REFERENCE COUNT: 110 THERE ARE 110 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

TITLE: Effect of a proton-donating solvent on complexation of classical and nonclassical porphyrins in a pyridine medium

AUTHOR(S): Berezin, D. B.; Toldina, O. V.

CORPORATE SOURCE: Russia

SOURCE: Zhurnal Neorganicheskoi Khimii (2002), 47(12), 2075-2081

PUBLISHER: MAI Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: Russian

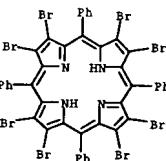
AB The inhibiting effect of proton-donating additives (HAc) on the rate of coordination of tetrabenzoporphine (I) and tetraphenyltetrabenzoporphine (I') as well as of N-substituted porphyrins (III and IV) with CuAc2 and ZnAc2 in a pyridine medium is shown. It is also shown that in the compds. I and II, the properties of the NH bond and the reactivity for a given reaction are close to those for nonclassical porphyrins (H2P). The N-substituted porphyrins III et IV do not behave the same way. The inhibition of the coordination reaction in the compound III and IV can be explained by the increase of basicity of the tertiary nitrogen atoms in these mols.

IT 131214-86-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (effect of a proton-donating solvent on complexation of classical and nonclassical porphyrins in a pyridine medium)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-(9Cl) (CA INDEX NAME)





L6 ANSWER 23 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2002:900049 CAPLUS

DOCUMENT NUMBER: 138:304092

TITLE: Photoinitiated olefin epoxidation with molecular oxygen, sensitized by free base porphyrins and promoted by hexacarbonylmolybdenum in homogeneous solution

AUTHOR(S): Campestrini, Sandro; Tonellato, Umberto

CORPORATE SOURCE: Universita di Padova, Dipartimento di Chimica  
Organica, Centro CNR di Studio sui Meccanismi di Reazioni Organiche, Padua, 35131, Italy

SOURCE: European Journal of Organic Chemistry (2002), (22), 3827-3832

CODEN: EJOCEK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:304092

AB The photooxidn. of various olefins in homogeneous solution under an oxygen atmospheric, by use of visible light, a dye sensitizer, and an oxygen-transfer

catalyst, has been investigated. The oxygen transfer from mol. oxygen to olefin involves the following steps: (i) photoinduced singlet-oxygen formation, (ii) alkyl hydroperoxide formation through the ene reaction, (iii) the intermediacy of a reactive molybdenum peroxide, and (iv) olefin epoxidn. of the remaining substrate or of a second olefin. Among the various sensitizers and catalysts tested the electron-deficient free base porphyrin 5,10,15,20-tetrakis(2',6'-dichlorophenyl)- $\beta$ -octabromoporphyrin and hexacarbonylmolybdenum showed the best performances in terms of robustness and activity. Under suitable conditions, complete olefin conversion can be obtained by adoption of molar ratios of sensitizer/catalyst/substrate of 1:50:2000, with the formation of the corresponding epoxide in up to 38% yield, which corresponds to 77% of the theor. maximum. Quite interestingly, olefins reluctant to undergo ene reactions may be epoxidized in the presence of a second sacrificial olefin, yielding the corresponding epoxides with up to 80% total selectivity.

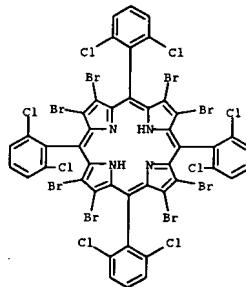
IT 107035-95-0

RL: RGT (Reagent); RACT (Reactant or reagent)  
(photoinitiated olefin epoxidn. with mol. oxygen sensitized by free base porphyrins and promoted by hexacarbonylmolybdenum)

RN 107035-95-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 23 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 24 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:808700 CAPLUS

DOCUMENT NUMBER: 138:73108

TITLE: On the role of  $\beta$ -fluorine substitution on the extent of core deformation of porphyrin dications

AUTHOR(S): Porhier, Emmanuel; Toupet, Loïc; Leroy, Jacques;

CORPORATE SOURCE: Laboratoire de Chimie Organometallique et Biologique, Université de Rennes 1, UMR CNRS 6509, Rennes, F-35042, Fr.

SOURCE: Tetrahedron Letters (2002), 43(46), 8293-8296

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Careful anal. of fully and partially  $\beta$ -fluorinated dicationic porphyrins have been performed suggesting an electronic influence of the  $\beta$ -fluorine atoms on the extent of the macrocycle deformation, in agreement with the crystal structure of  $\beta$ -octafluoro-meso-tetraphenylporphyrin dication.

IT 479637-18-6

RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation) (crystal structure; role of  $\beta$ -fluorine substitution on the extent of core deformation of porphyrin dications)

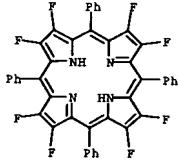
RN 479637-18-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl-, diperchlorate, compd. with dichloromethane (1:2), dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 186885-28-9

CMF C44 H22 F8 N4



CM 2

CRN 7601-90-3

CMF C1 H 04



L6 ANSWER 24 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CM 3

CRN 75-09-2

CMF C H2 Cl2

Cl-CH2-Cl

IT 479637-13-3 479637-15-5

RL: PRP (Properties)  
(role of  $\beta$ -fluorine substitution on the extent of core deformation of porphyrin dications)

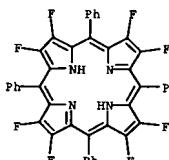
RN 479637-13-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 186885-28-9

CMF C44 H22 F8 N4



CM 2

CRN 7601-90-3

CMF C1 H 04



RN 479637-15-5 CAPLUS

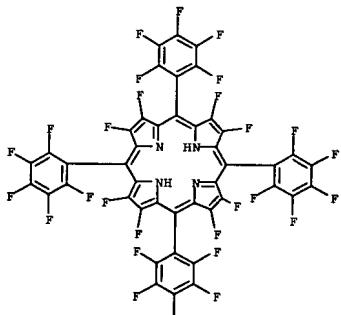
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraakis(pentafluorophenyl)-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 121399-88-0

CMF C44 H2 F28 N4

PAGE 1-A



PAGE 2-A

CM 2  
CRN 7601-90-3  
CMF Cl H O4

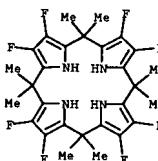


REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 25 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2002:751572 CAPLUS  
DOCUMENT NUMBER: 137:389723  
TITLE: Theoretical Study of Anion Binding to Calix[4]pyrrole: the Effects of Solvent, Fluorine Substitution, Cosolute, and Water Traces  
AUTHOR(S): Blas, J. Ramon; Marquez, Manuel; Sessler, Jonathan L.; Luque, F. Javier; Orozco, Modesto  
CORPORATE SOURCE: Departament de Bioquímica i Biologia Molecular, Facultat de Química, Universitat de Barcelona, Barcelona, 08028, Spain  
SOURCE: Journal of the American Chemical Society (2002), 124(43), 12796-12805  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The binding of different anions to calix[4]pyrrole has been studied by means of mol. dynamics coupled to thermodyn. integration calcs. The effect of different apolar solvents, octafluoro substitution, and the change in binding free energy derived from the presence of cosolute and water traces (the hydrated salt used to introduce the anion in the solution) were examined. Calcs. allow us to rationalize the differential binding of ions to calix[4]pyrrole and octafluorocalix[4]pyrrole as well as to predict the behavior in new solvents for which exptl. data are not available yet. It is found that both calix[4]pyrrole and octafluorocalix[4]pyrrole have a dramatic preference for F- in the gas phase and pure aprotic solvents, but the situation can change dramatically in protic solvents or in the presence of the hydrated cation which is used as cosolute of the anion. Overall, our results provide interesting clues for a better understanding of the process detected exptl. as "binding".

IT 311804-81-6  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)  
(effects of solvents and fluorine substitution on anion binding to calix[4]pyrrole from mol. dynamics and thermodyn. integration)  
RN 311804-81-6 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



IT 475644-56-5  
RL: FNU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)  
(optimized mol. structure of chloride-octafluorocalix[4]pyrrole, fluoride- calix[4]pyrrole, phosphate-calix[4]pyrrole, and fluoride-tetrabutylammonium trihydrate complexes)  
RN 475644-56-5 CAPLUS

L6 ANSWER 25 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2002:749114 CAPLUS  
DOCUMENT NUMBER: 138:48962

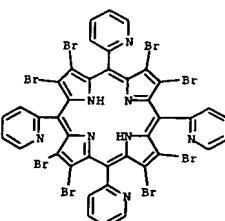
TITLE: Perhalogenated 2-pyridylporphyrin complexes: synthesis, self-coordinating aggregation properties, and catalytic studies  
AUTHOR(S): Reboucas, Julio S.; De Carvalho, Maria Eliza M. D.; Idemori, Ynara M.  
CORPORATE SOURCE: Departamento de Química - ICEX - Universidade Federal de Minas Gerais, Belo Horizonte, 31270-901, Brazil  
SOURCE: Journal of Porphyrins and Phthalocyanines (2002), 6(1), 50-57  
PUBLISHER: Society of Porphyrins & Phthalocyanines  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 138:48962

AB The synthesis of 2,3,7,8,12,13,17,18-octabromo-meso-tetrakis(2-pyridyl)porphyrin, H2Br8T2PyP, is described, including the comparison of four attempted methods for the demetalation of ZnBr8T2PyP. One of the methods represents a strategy of demetalation based on the acid-base properties of the macrocycle, the solvent-dependent kinetics of metal insertion into porphyrins and the pH-dependent solubility of the 2-pyridylporphyrin derivs. in water. Self-coordinating aggregation of ZnBr8T2PyP in non-coordinating solvents was verified by 1H NMR spectroscopy. The Mn(III)/Mn(II) redox potential for MnBr8T2PyP is 0.38 V higher than the reduction potential measured for its 1st-generation analog, MnT2PyP.

Cyclohexane hydroxylation by iodosylbenzene was performed in CH3CN catalyzed by MnBr8T2PyP and MnT2PyP. MnBr8T2PyP was highly active, even at low concentration (5 + 10-5 M), but perhalogenation did not account for oxidative robustness. At such a low catalyst concentration, MnT2PyP exhibited no activity as inferred by comparison to blank expts.

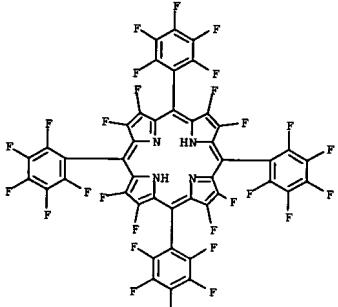
IT 478363-47-2  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(reactant for preparation of manganese perhalogenated tetrakis(pyridyl)porphyrinato complexes)

RN 478363-47-2 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetra-2-pyridinyl- (9CI) (CA INDEX NAME)



L6 ANSWER 27 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 2002:725874 CAPLUS  
 138:49060  
 TITLE: Synthesis of F28 tetraphenylporphyrin and its application to the separation and detection of lithium (I)  
 AUTHOR(S): Koyanagi, Kenji; Tabata, Masaaki  
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, 1-Honjo-machi, Saga-shi, Saga, 840-8502, Japan  
 SOURCE: Bunseki Kagaku (2002), 51(9), 803-807  
 CODEN: BNSKAKI ISSN: 0525-1931  
 PUBLISHER: Nippon Bunseki Kagakkai  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Japanese  
 AB 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin (F28 tetraphenylporphyrin, OTFPP) was synthesized by the condensation of 3,4-difluoropyrrole and pentafluorobenzaldehyde. 3,4-Difluoropyrrole was prepared from 2,2,3,3-tetrafluorosuccinic acid as the starting material through 5-step reaction processes. The acid-dissociation consts. of OTFPP were determined by a solvent-extraction method in the presence of tetrabutylammonium chloride (0.1 mol dm<sup>-3</sup>). The 28 fluorine atoms decreased the basicity of the porphyrin and made two protons of imidazoles release at pH 4 and 7 ([H<sup>+</sup>]<sub>o</sub> + Na<sup>+</sup> .dblhaw. [(H<sup>+</sup> - Na<sup>+</sup>)<sub>o</sub>, pKa3 4.2] + Na<sup>+</sup> .dblhaw. [(F<sup>2+</sup> - Na<sup>+</sup>)<sub>o</sub>, pKa4 8.0]). The protons of the tetraphenylporphyrin unsubstituted by fluorine atom did not dissociate at a pH lower than 14. OTFPP reacted with lithium ion in the neutral pH range, and gave a new absorption spectrum with a maximum wavelength of 416 nm in chloroform.  
 IT 121399-88-0  
 RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of F28 tetraphenylporphyrin and separation and detection of lithium)  
 RN 121399-88-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (SCI) (CA INDEX NAME)

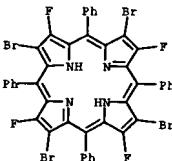
PAGE 1-A



PAGE 2-A

|  
F

L6 ANSWER 28 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 2002:641275 CAPLUS  
 137:379220  
 TITLE: Synthesis and characterization of partially  $\beta$ -fluorinated 5,10,15,20-tetraphenylporphyrins and some derivatives  
 AUTHOR(S): Leroy, Jacques; Porbier, Emmanuel; Bondor, Arnaud  
 CORPORATE SOURCE: UMR CNRS 8640, Departement de Chimie, Ecole Normale Supérieure, Paris, 75231, Fr.  
 SOURCE: Tetrahedron (2002), 58(33), 6713-6722  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 137:379220  
 AB The synthesis of partially  $\beta$ -fluorinated meso-tetraphenylporphyrins using Lindsey conditions, was examined, starting either from 3,4-difluoro-1H-pyrrole or from 3-fluoro-1H-pyrrole. In the case of the 1st synthon, condensation with pyrrole and benzaldehyde afforded a mixture of porphyrins of general formula  $\beta$ -FnTPP ( $n = 0, 2, 4, 6, 8$ ) displaying linearly correlated spectroscopic and electrochem. properties. With the 2nd synthon, condensation with benzaldehyde produced an irresolvable mixture of  $\beta$ -tetrafluoroporphyrins presenting spectroscopic and electrochem. properties in coherence with those observed in the 1st case. Preliminarily, the synthesis and isolation of the hitherto unknown 3-fluoro-1H-pyrrole was approached via several methods. Preparation of zinc complexes of the fluorinated porphyrins is reported.  
 IT 475561-96-7P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of partially  $\beta$ -fluorinated porphyrins and their zinc complexes)  
 RN 475561-96-7 CAPLUS  
 CN 21H,23H-Porphine, 2,7,12,17-tetrabromo-3,8,13,18-tetrafluoro-5,10,15,20-tetraphenyl- (SCI) (CA INDEX NAME)



L6 ANSWER 29 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2002:638268 CAPLUS  
 DOCUMENT NUMBER: 137:185360

TITLE: Preparation, binding properties, and uses of halogenated calixpyrroles, calixpyridinopyrroles and calixpyridines  
 INVENTOR(S): Sessler, Jonathan L.; Marquez, Manuel; Anzenbacher, Pavel; Shriner, James A.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 104 pp., Cont.-in-part of U.S. Ser. No. 838,998.  
 CODEN: USXKCO

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002115566	A1	20020822	US 2001-939514	20010824
CA 2391030	AA	19971016	CA 1997-2391030	19970404
US 6262257	B1	20010717	US 1997-833379	19970404
US 2002026047	A1	20020228	US 2001-838998	20010420
WO 2003018548	A2	20030306	WO 2002-US27252	20020826
WO 2003018548	A3	20030703		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MX, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TI, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BE, BJ, CF, CG, CL, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			US 1996-149509	P 19960405
			US 1996-242039	P 19960827
OTHER SOURCE(S):	MARPAT 137:185360		US 1996-266949	P 19960925
GI			US 1996-33395P	P 19961217
			US 1996-33396P	P 19961217
			US 1997-833379	A3 19970404
			US 2001-838998	A2 20010420
			CA 1997-2251072	A3 19970404
			US 2001-939514	A 20010824

Chemical structures I and II are shown. Structure I is a calixpyridine macrocycle with four phenyl groups at the 1, 4, 9, and 12 positions. Structure II is a calixpyridinopyrrole macrocycle with two phenyl groups at the 1, 4, 9, and 12 positions.

I  
 II

L6 ANSWER 29 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

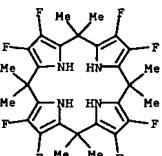
AB Halogenated calixpyrrole, calixpyridinopyrrole, and calixpyridine macrocycles, such as octabromo-meso-octamethylcalix[4]pyrrole (I) and calixpyridinopyrrole II, having 4-12 pyrrolic rings with greater stability were prepared for uses such as dialysis, ion exchange, and environmental remediation. Thus, I was prepared in 90% yield by bromination of the corresponding meso-octamethylcalix[4]pyrrole using N-bromosuccinimide in THF. Enhanced anion, neutral mol. binding affinity and different binding selectivities as compared to their nonhalogenated congeners as judged from <sup>1</sup>H NMR, <sup>19</sup>F NMR and fluorescence emission spectroscopic analyses.

IT 311804-81-6P  
 RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PVP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(calixpyrrole and anion binding properties of calixpyrroles, calixpyridinopyrroles and calixpyridines for use environmental remediation, kidney dialysis and cation exchangers)

RN 311804-81-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



IT 190517-33-0P

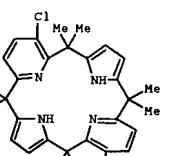
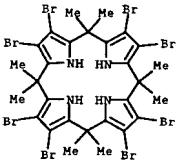
RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PVP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation and anion binding properties of calixpyrroles, calixpyridinopyrroles and calixpyridines for use environmental remediation, kidney dialysis and cation exchangers)

RN 190517-33-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)

L6 ANSWER 29 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L6 ANSWER 30 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:626618 CAPLUS

DOCUMENT NUMBER: 139:197287

TITLE: Lewis-base binding properties of free-base  $\beta$ -octahalotetraphenylporphyrins. (Erratum to document cited in CA137:279005)

AUTHOR(S): Bhayappa, P.; Bhavana, P.

CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Chennai, 600 036, India

SOURCE: Chemical Physics Letters (2002), 360 (5,6), 592

CODEN: CPHLBC; ISSN: 0009-2614

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the Abstract, line 2, "The kinetics of base..." should be "The base...". On page 108, paragraph 3, line 9, "The kinetics of anion..." should be "The anion...". On page 109, paragraph 1, lines 4 and 5, "nitrogenous bases, kinetics of base..." should be "nitrogenous bases, base...".

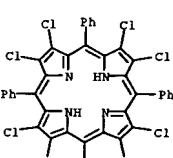
IT 120644-25-9, 2,3,7,8,12,13,17,18-Octachloro-5,10,15,20-tetraphenylporphyrin 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(binding with Lewis acid bases; Lewis-base binding properties of free-base  $\beta$ -octahalotetraphenylporphyrins (Erratum))

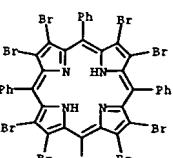
RN 120644-25-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS

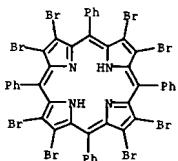
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



IT 465536-78-1P 465536-80-5P 465536-81-6P  
 465536-84-9P 465536-87-2P 465536-90-7P  
 465536-91-8P 465536-92-9P 465536-93-0P  
 465536-95-2P 465536-96-3P 465536-97-4P  
 465536-98-5P 465536-99-6P 465537-00-2P  
 465537-01-3P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process);  
 (preparation of, formation consts. for; Lewis-base binding properties of  
 free-base  $\beta$ -octahalotetraphenylporphyrins (Erratum))  
 RN 465536-78-1 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,  
 compd. with quinoline (1:1) (9CI) (CA INDEX NAME)

CM 1

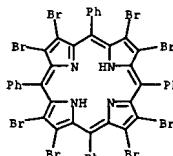
CRN 131214-86-3  
CMF C44 H22 Br8 N4

CM 2

CRN 91-22-5  
CMF C9 H7 N

RN 465536-80-5 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,  
 compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

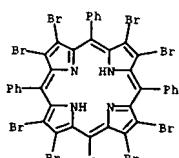
CRN 131214-86-3  
CMF C44 H22 Br8 N4

CM 2

CRN 110-86-1  
CMF C5 H5 N

RN 465536-81-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,  
 compd. with 3-methylpyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

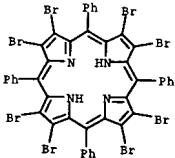
CRN 131214-86-3  
CMF C44 H22 Br8 N4

CM 2

CRN 108-99-6  
CMF C6 H7 N

RN 465536-84-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,  
 compd. with 1-methyl-1H-imidazole (1:1) (9CI) (CA INDEX NAME)

CM 1

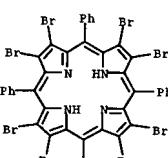
CRN 131214-86-3  
CMF C44 H22 Br8 N4

CM 2

CRN 616-47-7  
CMF C4 H6 N2

RN 465536-87-2 CAPLUS  
 CN 4-Pyridinamine, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octabromo-  
 5,10,15,20-tetraphenyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

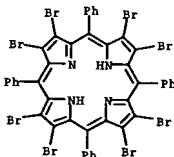
CRN 131214-86-3  
CMF C44 H22 Br8 N4

CM 2

CRN 1122-58-3  
CMF C7 H10 N2

RN 465536-90-7 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,  
 compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3  
CMF C44 H22 Br8 N4

CM 2

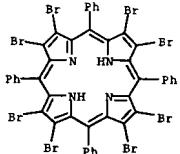
CRN 110-89-4  
CMF C5 H11 N



RN 465536-91-8 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,  
 compd. with 1,4-dioxane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3  
 CMF C44 H22 Br8 N4



CM 2

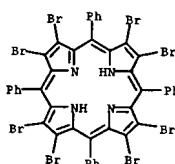
CRN 123-91-1  
 CMF C4 H8 O2



RN 465536-92-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,  
 compd. with sulfinylbis[methane] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3  
 CMF C44 H22 Br8 N4



CM 2

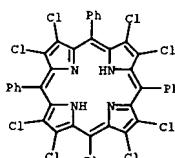
CRN 67-68-5  
 CMF C2 H6 O S



RN 465536-93-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,  
 compd. with quinoline (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9  
 CMF C44 H22 Cl8 N4



CM 2

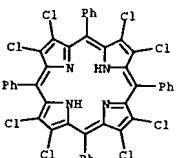
CRN 91-22-5  
 CMF C9 H7 N



RN 465536-95-2 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,  
 compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9  
 CMF C44 H22 Cl8 N4



CM 2

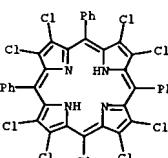
CRN 110-86-1  
 CMF C5 H5 N



RN 465536-96-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,  
 compd. with 3-methylpyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9  
 CMF C44 H22 Cl8 N4



CM 2

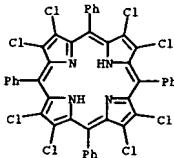
CRN 108-99-6  
 CMF C6 H7 N



RN 465536-97-4 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,  
 compd. with 1-methyl-1H-imidazole (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9  
 CMF C44 H22 Cl8 N4



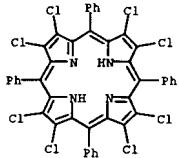
CM 2

CRN 616-47-7  
 CMF C4 H6 N2



RN 465536-98-5 CAPLUS  
CN 4-Pyridinamine, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9  
CMF C44 H22 C18 N4

CM 2

CRN 1122-58-3  
CMF C7 H10 N2

RN 465536-99-6 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

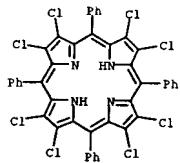
CM 1

CRN 120644-25-9  
CMF C44 H22 C18 N4

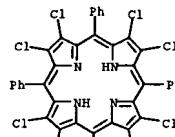
L6 ANSWER 30 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 465537-01-3 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with sulfinylbis(methane) (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9  
CMF C44 H22 C18 N4

CM 2

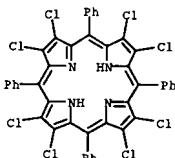
CRN 67-68-5  
CMF C2 H6 O S

CM 2

CRN 110-89-4  
CMF C5 H11 N

RN 465537-00-2 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with 1,4-dioxane (1:1) (9CI) (CA INDEX NAME)

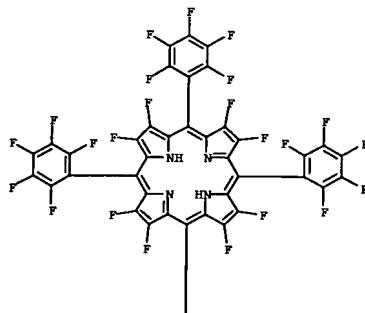
CM 1

CRN 120644-25-9  
CMF C44 H22 C18 N4

CM 2

CRN 123-91-1  
CMF C4 H8 O2

L6 ANSWER 31 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2002:626587 CAPLUS  
DOCUMENT NUMBER: 137:352662  
TITLE: Theoretical studies on the structural change of the N-protonated tetraphenylporphyrin. (II) - effects of the substituting fluorine groups  
AUTHOR(S): Huang, Xiao-Fen; Ma, Si-Yu; Liu, Ru-Zhuang  
CORPORATE SOURCE: Department of Chemistry, Beijing Normal University, Beijing, 100875, Peop. Rep. China  
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2002), 23(8), 1562-1566  
PUBLISHER: Gaodeng Jiaoyu Chubanshe  
DOCUMENT TYPE: Journal  
LANGUAGE: Chinese  
AB With the symmetry being reasonably restricted, the semi-empirical method of AM1 MO is used to calculate the geometries of 5,10,15,20-tetrakis(pentafluorophenyl)porphyrin (TF5PFH2) and 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin (F28TPH2) and their N-protonated diacids (TF5PFH2+4 and F28TPH2+4) which are kinds of important porphyrin derivs. Also, the configurational change in protonation process and the probable influence to mol. aggregation conducted by the change are discussed by the means of structure anal., population anal. and frontier orbital anal.  
IT 474422-37-2  
RL: FMU (Formation, unclassified); PPR (Properties); FORM (Formation, nonpreparative)  
(ther. studies on fluorine substituent effects on structural changes by N-protonation of tetraphenylporphyrin)  
RN 474422-37-2 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)-, conjugate diacid (9CI) (CA INDEX NAME)



PAGE 2-A

●2 H<sup>+</sup>

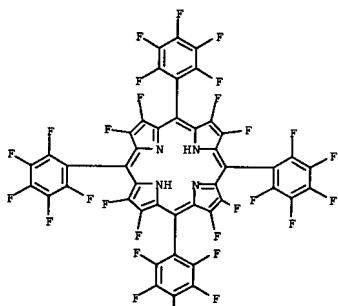
IT 121399-88-0

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (theor. studies on fluorine substituent effects on structural changes by N-protonation of tetraphenylporphyrin)

RN 121399-88-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



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L6 ANSWER 32 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2002:624523 CAPLUS  
DOCUMENT NUMBER: 139:220923  
TITLE: Unusual solvent dependent optical absorption spectral properties of free base perhaloporphyrins. [Erratum to document cited in CA135:263667]

AUTHOR(S): Bhyrappa, P.; Bhavana, P.  
CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Madras, Chennai, 600 036, India  
SOURCE: Chemical Physics Letters (2002), 360(5,6), 592  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal

LANGUAGE: English  
AB In Table 3, last data line, H2OETPP should be H2TPP. On page 43, paragraph 4, line 2, 1.70 should be -1.70; in line 3, 0.1 should be -0.10.

IT 120644-25-9, 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-

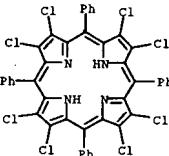
S,10,15,20-tetr phenyl- 131214-86-3, 2,3,7,8,12,13,17,18-

Octabromo-5,10,15,20-tetr phenylporphyrin  
RL: PRP (Properties)

(unusual solvent dependent optical absorption spectral properties of free-base perhaloporphyrins (Erratum))

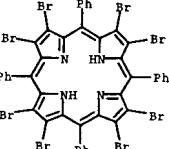
RN 120644-25-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetr phenyl- (9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetr phenyl- (9CI) (CA INDEX NAME)



L6 ANSWER 33 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2002:424652 CAPLUS  
DOCUMENT NUMBER: 137:155101  
TITLE: Catalytic Oxidations of Steroid Substrates by Artificial Cytochrome P-450 Enzymes  
AUTHOR(S): Yang, Jerry; Gabriele, Bartolo; Belvedere, Sandro; Hsing, Ying; Baslow, Ronald  
CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027, USA  
SOURCE: Journal of Organic Chemistry (2002), 67(15), 5057-5067  
PUBLISHER: CODEN: JOCERA; ISSN: 0022-3263  
DOCUMENT TYPE: American Chemical Society  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 137:155101

AB Catalysts comprising manganese-porphyrins carrying cyclodextrin binding groups are able to perform hydroxylations with substrate selectivity and regio- and stereoselectivity and high catalytic turnovers. The geometries of the catalyst/substrate complexes override intrinsic substrate reactivities, permitting attack on geometrically accessible saturated carbons

of steroids in the presence of secondary carbinol groups and carbon-carbon double bonds, as in enzymic reactions. Selective hydroxylations of steroid carbon 9 positions are of particular practical interest.

IT 161405-60-3P, 2,3,7,8,12,13,17,18-Octachloro-5,10,15,20-Tetrakis(4-mercaptop-2,3,5,6-tetrafluorophenyl)porphyrin

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); (regio- and stereoselective catalytic oxidns. of steroids by catalysts comprising manganese-porphyrins bound to cyclodextrins)

RN 161405-60-3 CAPLUS

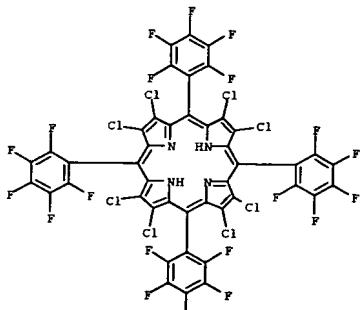
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 33 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PAGE 1-A



ACCESSION NUMBER: 2002:338995 CAPLUS  
DOCUMENT NUMBER: 1371279005

TITLE: Lewis-base binding properties of free-base  $\beta$ -octahalotetraphenylporphyrins

AUTHOR(S): Bhryappa, P.; Bhavana, P.  
CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Chennai, 600 036, India

SOURCE: Chemical Physics Letters (2002), 357(1,2), 108-112

CODEN: CPHLBC ISSN: 0009-2614

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Sym. substituted perhaloporphyrins, 2,3,7,8,12,13,17,18-octabromo (bromo and chloro)-5,10,15,20-tetraphenylporphyrins (H2OBTPP and H2OCTPP) have been examined as receptors for binding to Lewis bases. The kinetics of base binding to haloporphyrins showed an enhanced binding const. for H2OBTPP relative to H2OCTPP and follows a linear trend with increase in pKa values of the bases. The binding of Lewis-bases to perhaloporphyrin core is largely influenced by the extent of nonplanarity of the porphyrin core than the electron-withdrawing ability of the substituents. The higher binding const. of H2OBTPP relative to H2OCTPP have been interpreted in terms of greater nonpolarity of the former than the latter.

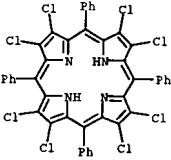
IT 120644-25-9, 2,3,7,8,12,13,17,18-Octachloro-5,10,15,20-tetraphenylporphyrin 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-

5,10,15,20-tetraphenylporphyrin

RL: CFS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (binding with Lewis acid bases; Lewis-base binding properties of free-base  $\beta$ -octahalotetraphenylporphyrins)

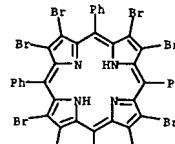
RN 120644-25-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



IT 465536-78-10 465536-80-5P 465536-81-6P  
465536-84-9P 465536-87-2P 465536-90-7P  
465536-91-8P 465536-92-9P 465536-93-0P  
465536-95-2P 465536-96-3P 465536-97-4P  
465536-98-5P 465536-99-6P 465537-00-2P  
465537-01-3P

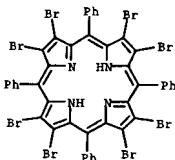
RL: CFS (Chemical process); PEP (Physical, engineering or chemical process); SPP (Synthetic preparation); PREP (Preparation); PROC (Process) (preparation of, formation const. for, Lewis-base binding properties of free-base  $\beta$ -octahalotetraphenylporphyrins)

RN 465536-78-1 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with quinoline (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3  
CMF C44 H22 Br8 N4



CM 2

CRN 91-22-5  
CMF C9 H7 N

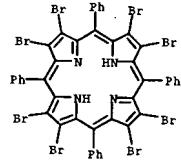


RN 465536-80-5 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3  
CMF C44 H22 Br8 N4



CM 2

CRN 110-86-1  
CMF C5 H5 N

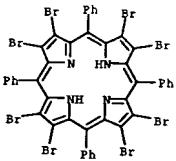


RN 465536-81-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with 3-methylpyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3  
CMF C44 H22 Br8 N4



CM 2

CRN 108-99-6

CMF C6 H7 N

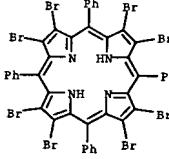


RN 465536-84-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with 1-methyl-1H-imidazole (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3  
CMF C44 H22 Br8 N4



CM 2

CRN 616-47-7  
CMF C4 H6 N2

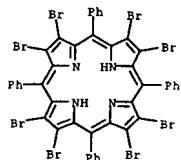


RN 465536-87-2 CAPLUS

CN 4-Pyridinamine, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

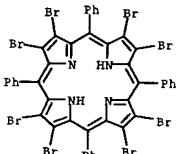
CRN 131214-86-3  
CMF C44 H22 Br8 N4



CM 2

CRN 1122-58-3  
CMF C7 H10 N2RN 465536-90-7 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

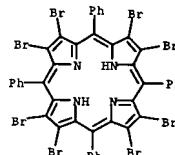
CM 1

CRN 131214-86-3  
CMF C44 H22 Br8 N4

CM 2

CRN 110-89-4  
CMF C5 H11 NRN 465536-91-8 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with 1,4-dioxane (1:1) (9CI) (CA INDEX NAME)

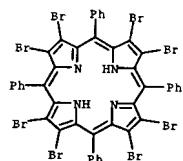
CM 1

CRN 131214-86-3  
CMF C44 H22 Br8 N4

CM 2

CRN 123-91-1  
CMF C4 H8 O2RN 465536-92-9 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with sulfinylbis[methane] (1:1) (9CI) (CA INDEX NAME)

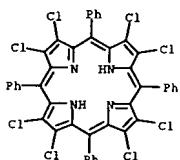
CM 1

CRN 131214-86-3  
CMF C44 H22 Br8 N4

CM 2

CRN 67-68-5  
CMF C2 H6 O SRN 465536-93-0 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with quinoline (1:1) (9CI) (CA INDEX NAME)

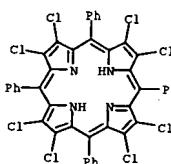
CM 1

CRN 120644-25-9  
CMF C44 H22 Cl8 N4

CM 2

CRN 91-22-5  
CMF C9 H7 NRN 465536-95-2 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

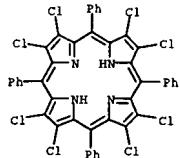
CRN 120644-25-9  
CMF C44 H22 Cl8 N4

CM 2

CRN 110-86-1  
CMF C5 H5 NRN 465536-96-3 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with 3-methylpyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

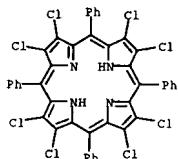
CRN 120644-25-9  
CMF C44 H22 Cl8 N4



CM 2

CRN 108-99-6  
CMF C6 H7 NRN 465536-97-4 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with 1-methyl-1H-imidazole (1:1) (9CI) (CA INDEX NAME)

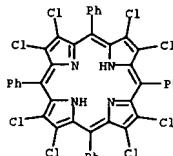
CM 1

CRN 120644-25-9  
CMF C44 H22 C18 N4

CM 2

CRN 616-47-7  
CMF C4 H6 N2RN 465536-98-5 CAPLUS  
CN 4-Pyridinamine, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

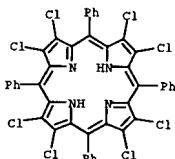
CM 1

CRN 120644-25-9  
CMF C44 H22 C18 N4

CM 2

CRN 1122-58-3  
CMF C7 H10 N2RN 465536-99-6 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

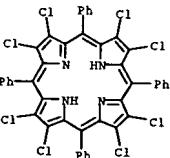
CM 1

CRN 120644-25-9  
CMF C44 H22 C18 N4

CM 2

CRN 110-89-4  
CMF C5 H11 NRN 465537-00-2 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with 1,4-dioxane (1:1) (9CI) (CA INDEX NAME)

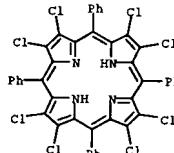
CM 1

CRN 120644-25-9  
CMF C44 H22 C18 N4

CM 2

CRN 123-91-1  
CMF C4 H8 O2RN 465537-01-3 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with sulfinylbis[methane] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9  
CMF C44 H22 C18 N4

CM 2

CRN 67-68-5  
CMF C2 H6 O S

REFERENCE COUNT:

27

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2002:337886 CAPLUS

DOCUMENT NUMBER: 137:194452

**TITLE:** Immobilization of  $\beta$  halogenated ironporphyrin in the silica matrix by the sol-gel process  
**AUTHOR(S):** Aparecida Vidotto, Ednalyva, Silvia Monsalves Moreira, Maria da Silva Vinhado, Fabio Ciuffi, Katia Jorge, Rangel Nascimento, Otaciro, Yamamoto, Yassuko  
**CORPORATE SOURCE:** Departamento de Quimica, Otaciro, Yamamoto, FFCLRP, Ribeirao Preto, SP, 14040-901, Brazil  
**SOURCE:** Journal of Non-Crystalline Solids (2002), 304(1-3), 151-159

CODEN: JNCSEB; ISSN: 0022-3093

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

**AB** The authors present the synthesis and characterization of a hybrid organic-inorg. material using robust metalloporphyrins halogenated in both meso and  $\beta$ -position, the iron complexes of 5,10,15,20-tetrakis(pentafluorophenyl)porphyrin and 2,3,7,8,12,13,17,18-octa- $\beta$ -bromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin, which stabilize the porphyrin against oxidative degradation. The immobilization was developed by the sol-gel process using pyridine and imidazole as template. EPR spectra of the iron complex of 2,3,7,8,12,13,17,18-octa- $\beta$ -bromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin show that the entrapment of ironporphyrin is in a higher symmetry compared to the systems in solution. A reduction of iron was observed in the presence of imidazole, determined by the absence of an EPR spectrum. The addition of chlorhydric acid vapor induced an oxidation of iron and a small quantity of iron in a high spin state was detected by a component with axial symmetry. The ironporphyrins were active as catalysts for cyclooctene epoxidation using iodosylbenzene and hydrogen peroxide as oxygen donors. The perhalogenated porphyrins immobilized had a smaller activity due to their iron oxidation and spin states.

IT 139944-26-6P, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-

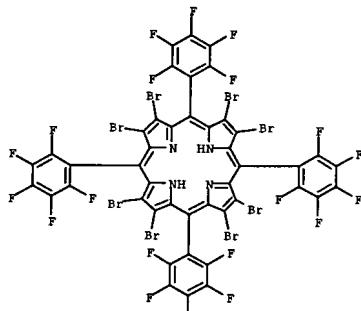
tetrakis(pentafluorophenyl)porphyrin

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate); preparation of hybrid organic-inorg. materials of iron metalloporphyrins halogenated in meso and  $\beta$ -positions immobilized in silicon matrix by sol-gel process)

RN 139944-26-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

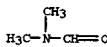


PAGE 2-A

REFERENCE COUNT:

64

THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

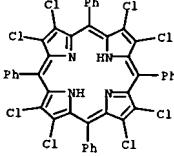
CRN 68-12-2  
CMF C3 H7 N O

IT 120644-25-P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation, electronic spectra, redox potentials and complexation with terbium(III))

RN 120644-25-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

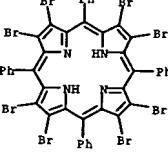


IT 131214-86-3P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation, mol. structure, electronic spectra, redox potentials and complexation with terbium(III))

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

88

THERE ARE 88 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2002:308212 CAPLUS

137:10848

**TITLE:** Comparative Study of Structure-Properties Relationship for Novel  $\beta$ -Halogenated Lanthanide Porphyrins and Their Nickel and Free Bases Precursors, as a Function of Number and Nature of Halogens Atoms

**AUTHOR(S):** Spyroulias, G. A.; Despotopoulos, A. P.; Raptopoulou, C. P.; Terzis, A. I.; de Montaizon, D.; Poilblanc, R.; Coutsolelos, A. G.

**CORPORATE SOURCE:** Department of Chemistry Laboratory of Bioinorganic Coordination Chemistry School of Science, University of Crete, Heraklion, Crete, 714 09, Greece

Inorganic Chemistry (2002), 41(10), 2648-2659

CODEN: INOCAJ; ISSN: 0020-1669

American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:40848

**AB** The synthetic route of partially  $\beta$ -halogenated via a metal-assisted reaction and perhalogenated Tb complexes is described. This protocol allows the facile insertion of the halogens (bromines or chlorides) to the porphyrin peripheral positions. The electronic absorption spectra and the redox potentials of the free porphyrins as well as the Tb complexes are dramatically affected as the number of halogen atoms increase. In fact, two antagonistic effects are responsible for that, the inductive and the distortion effects on the porphyrin ring. They result in a red shift for the Soret band and a stabilization/destabilization of the HOMOs/LUMOs which is turn is manifested by variations on the redox potentials. The new crystal structure of the Ni(C18TPP) is discussed in great detail and compared with the previously reported structures of Tb(C18TPP)(OAc)(DMSO)2-3PhCH3-MeOH and H2(Br8TPP), as well as with other perhalogenated Ni porphyrins available in the literature.

IT 189874-66-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure)

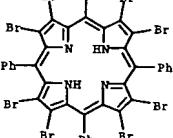
RN 189874-66-6 CAPLUS

CN Formamide, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-21H,23H-porphine (2:1) (9CI) (CA INDEX NAME)

CH 1

CRN 131214-86-3

CMF C44 H22 Br8 N4



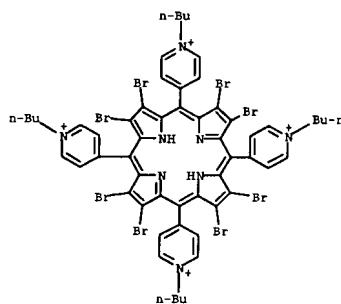
CH 2

CRN 131214-86-3

CMF C44 H22 Br8 N4

L6 ANSWER 37 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2002218837 CAPLUS  
 DOCUMENT NUMBER: 137:5840  
 TITLE: Catalytic activity of tetraarylporphyrins in the oxidation reactions of saturated hydrocarbons  
 AUTHOR(S): Avdeev, M. V.; Bagrii, E. I.; Maravin, G. B.; Korolev, Yu. M.  
 CORPORATE SOURCE: Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Moscow, 117912, Russia  
 SOURCE: Kinetics and Catalysis (Translation of Kinetika i Kataliz) (2002), 43(1), 38-44  
 PUBLISHER: MAIK Nauka/Interperiodica Publishing  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 137:5840  
 AB Conference proceedings. The oxidation of cyclic hydrocarbons by potassium peroxymonosulfate catalyzed by the iron and manganese complexes of tetra-(4-N-butylpyridinium)porphyrin, tetraphenylporphyrin, and mixed porphyrins containing Ph and butylpyridyl substituents was studied in an aqueous acetonitrile medium. The test catalysts were dissolved in the reaction medium or adsorbed on layered aluminosilicates. It was found that the immobilization of metal complexes on layered aluminosilicates, as well as the bromination of porphyrins, decreased the activity of catalysts in a number of cases, although it improved their stability. The addition of pyridine in an equimolar amount with respect to metal complexes to the reaction mixture increased the activity of dissolved manganese complexes. An increase in the number of butylpyridyl meso-substituents in a porphyrin mol. improved the catalytic activity of a metal complex.  
 IT 432028-75-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (Catalytic activity of tetraarylporphyrins in the oxidation reactions of saturated hydrocarbons)  
 RN 432028-75-6 CAPLUS  
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[1-butyl-, tetrapерchlorate (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 432028-74-5  
 CMF C56 H54 Br8 N8

L6 ANSWER 37 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CM 2

CRN 14797-73-0  
 CMF Cl 04

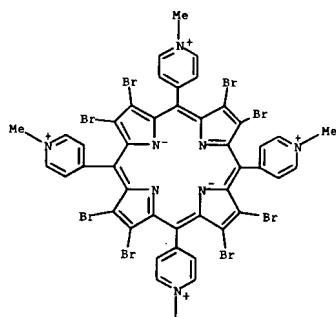


REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 38 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2002102603 CAPLUS  
 DOCUMENT NUMBER: 136:331159  
 TITLE: Kinetics of zinc ion incorporation in base into a centrally aprotic beta-octabrominated cationic water-soluble porphyrin and its monolithium complex  
 AUTHOR(S): Bailey, Sabrina L.; Hambright, P.  
 CORPORATE SOURCE: Department of Chemistry, Howard University, Washington, DC, 20059, USA  
 SOURCE: Journal of Porphyrins and Phthalocyanines (2001), 5(12), 829-834  
 PUBLISHER: John Wiley & Sons Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The kinetics of zinc incorporation from pH 12 to 13 into the centrally aprotic BrP(4)2+ form of beta-octabromo-meso-tetrakis[N-methyl-4-pyridyl]porphyrin and its monolithium complex were studied at 25.0°C, ionic strength ( $\bar{I}$ ) = 0.10. The reactions were first order in porphyrin and total zinc concns. For BrP(4)2+, the specific rate constant was  $5.1 \times 105$  M-1 s-1 for Zn(OH)2 aqueous 9.9  $\times 104$  M-1 s-1 for Zn(OH)3+, and Zn(OH)42- was unreactive. The Li-BrP(4)3+ complex had a formation constant with BrP(4)2+ of 1.1  $\times 103$  M-1 from both kinetic and equilibrium measurements. In solns. containing both BrP(4)2+ and Li-BrP(4)3+, zinc incorporation proceeded only through BrP(4)2+.  
 IT 413578-85-5  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRO (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
 (Kinetics of zinc ion incorporation in base into a centrally aprotic beta-octabrominated cationic water-soluble porphyrin and its monolithium complex)  
 RN 413578-85-5 CAPLUS  
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[1-methyl-, bis(inner salt) (9CI) (CA INDEX NAME)

L6 ANSWER 38 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2001:886633 CAPLUS

DOCUMENT NUMBER: 136:578

TITLE: Lithium detection in liquid biological samples and reagents therefor  
INVENTOR(S): Balazs, Nicholas Dennis Henry; Secombe, John William  
PATENT ASSIGNEE(S): Seba Diagnostics Pty. Ltd., Australia  
SOURCE: PCT Int. Appl., 41 pp.  
CODEN: PIXXD2DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
WO 2001092881	A1	20011206	WO 2001-AU603	20010525	
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, BY, KG, KZ, MD, RU, TZ, TM	RE:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW	AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG	2001-2409971	CA 2001-2409971
CA 2409971	AA	20011206	CA 2001-AU603	20010525	
EP 1283986	A1	20030219	EP 2001-933464	20010525	
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR	US 2003186450	A1	20031002	US 2003-296592	20030604
PRORITY APPLN. INFO.: AU 2000-7768	AU 2000-7768	A 20000526			
	WO 2001-AU603	W 20010525			

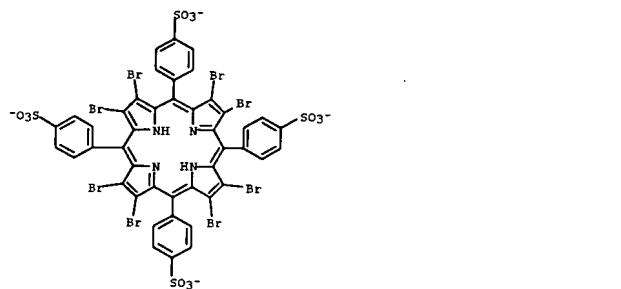
AB A method of detecting soluble lithium in a liquid biol. sample comprising combining: (a) an amount of the biol. sample; (b) 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl) porphyrin; (c) alkali; (d) detergent; (e) chelating agent; and (f) optionally a suitable solvent, to produce a test sample; detecting absorbance change of the test sample relative to a lithium deficient standard sample at a wavelength of between about 475nm and about 485nm, between about 515nm and about 525nm or simultaneously between about 475nm and about 485nm and between about 515nm and about 525nm, wherein absorbance change indicates presence of soluble lithium in the biol. sample. Also disclosed is a method of quant. measuring soluble lithium ions in a biol. sample and a reagent for use in such methods.

IT 176173-80-1

RL: ANT (Analyte); ANST (Analytical study)  
(lithium detection in liquid biol. samples and reagents therefor)

RN 176173-80-1 CAPLUS

CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis-, ion(4-) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2001:732629 CAPLUS

DOCUMENT NUMBER: 136:37433

TITLE: Structure and physicochemical properties of substituted porphyrins  
AUTHOR(S): Karmanova, T. V.; Gromova, T. V.; Berezin, B. D.; Semeikin, A. S.; Syrbu, S. A.  
CORPORATE SOURCE: Ivanovo State University of Chemical Engineering, Ivanovo, Russia  
SOURCE: Russian Journal of General Chemistry (Translation of Zhurnal Obozrhei Khimii) (2001), 71(5), 803-808

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Reactions of substituted porphyrins: 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrphenylporphine, 2,3,7,8,12,13,17,18-octamethyl-5,10,15,20-tetrphenylporphine, and dodecaphenylporphine with organic bases (pyridine, piperidine, DMF, DMSO) and acetic acid were studied by spectrophotometry. Acid-base interaction between porphyrins and organic bases and formation of ionic species in toluene solution containing an organic base were revealed

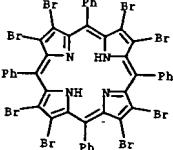
for the first time. The effect of electronic and structural factors on the acid-base interactions of porphyrin ligands with organic bases is discussed. The stability consts. were calculated for complexes of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrphenylporphine with organic bases, and electronic absorption spectra of substituted porphyrins in basic organic solvents were recorded.

IT 131214-86-3

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(structure and physicochem. properties of substituted porphyrins)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2001:536788 CAPLUS

DOCUMENT NUMBER: 136:74895

TITLE: Conformational analysis of octa- and tetrahalogenated tetraphenylporphyrins and their metal derivatives

AUTHOR(S): Gruden, M.; Grubisic, S.; Coutssolelos, A. G.; Niketic, S. R.

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, University of Belgrade, Belgrade, YU-11001, Yugoslavia

SOURCE: Journal of Molecular Structure (2001), 595(1-3), 209-224

PUBLISHER: JOMSB4; ISSN: 0022-2860

DOCUMENT TYPE: Elsevier Science B.V.

LANGUAGE: English

AB A new maximally diagonal force field for mol. modeling of metalloporphyrins is developed and optimized on the crystal structures of nickel(II)-porphyrin, nickel(II) mono-tert-butylporphyrin and nickel(II) di-tert-butylporphyrin. It is then used to investigate non-planar distortions of octa- and tetrachloro tetraphenylporphyrins (TTP) and their Ni(II) and Tb(III) complexes. Mol. mechanics (MM) calcs. reproduced very well the structure of Tb(III) octachloro-TTP (so far the only example of a crystallog. characterized chloro TTP metal derivative). Normal-coordinate structural decomposition (NSD) anal. was performed on the equilibrium structures

obtained by MM calcs. As expected, sad distortion dominates in octachloro structures irresp. of the presence or the size of the central metal atom; dom distortion dominates in tetrachloro structures with large Tb(III) central atom, while sad, ruf, wav and pro distortions are present in various amts. in other tetrachloro structures (TTP free base and Ni(II) complex) depending on the pattern of peripheral chloro substitution on the pyrrole rings. Other observed regularities are: reduction of the conformational

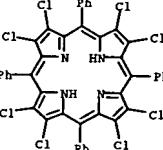
flexibility of the porphyrin core upon metalation, and increase of the dihedral angle between the Ph groups and the mean LSQ plane of the porphyrin core, as well as the overall increase in structural regularity upon the increase of the size of the central metal atom.

IT 120644-25-9

RL: PRP (Properties)  
(conformational anal. of octa- and tetrahalogenated tetraphenylporphyrins and metal derivs. with new maximally diagonal force field)

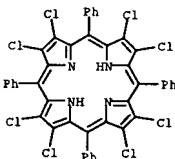
RN 120644-25-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrphenyl- (9CI) (CA INDEX NAME)

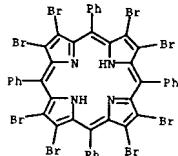


REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS

L6 ANSWER 42 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2001488195 CAPLUS  
DOCUMENT NUMBER: 135:263667  
TITLE: Unusual solvent dependent optical absorption spectral properties of free-base perhaloporphyrins  
AUTHOR(S): Bhayrappa, P.; Bhavana, P.  
CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Madras, Chennai, 600 036, India  
SOURCE: Chemical Physics Letters (2001), 342(1,2), 39-44  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A pair of free-base perhaloporphyrins, 2,3,7,8,12,13,17,18-octabromo- and octachloro-5,10,15,20-tetraphenylporphyrins (H2OETPP and H2OCTPP) were examined in solvents of varying polarity to delineate the effect of solvent on the optical absorption features. The perhaloporphyrins exhibit strong solvent-dependent absorption spectral features in contrast to 5,10,15,20-tetraphenylporphyrin, H2TPP. A dramatic red shift of Soret, B (>25 nm) and visible, Q (>50 nm) were observed for perhaloporphyrins in polar solvents relative to nonpolar solvents. This was ascribed to the enhanced distortion of the macrocyclic ring induced by H-bonding interaction between the porphyrin core pyrrolic N-H or pyrrolidine nitrogens with the solvent mols.  
IT 120644-25-9 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin  
RL: PRP (Properties)  
(unusual solvent dependent optical absorption spectral properties of free-base perhaloporphyrins)  
RN 120644-25-9 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



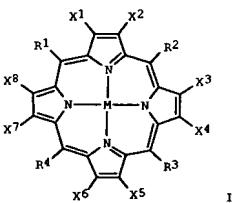
RN 131214-86-3 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

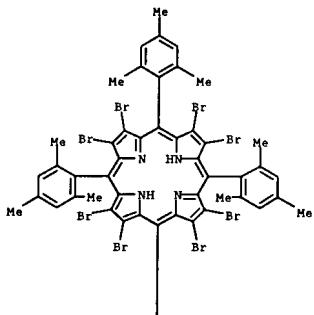
L6 ANSWER 43 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2001371490 CAPLUS  
DOCUMENT NUMBER: 134:359572  
TITLE: Recordable optical disk suitable for readout at 400-450 nm  
INVENTOR(S): Sasa, Noboru  
PATENT ASSIGNEE(S): Ricoh Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001138634	A2	20010522	JP 1999-322999	19991112
PRIORITY APPLN. INFO.:			JP 1999-322999	19991112
OTHER SOURCE(S):		MARPAT 134:359572		
G1				

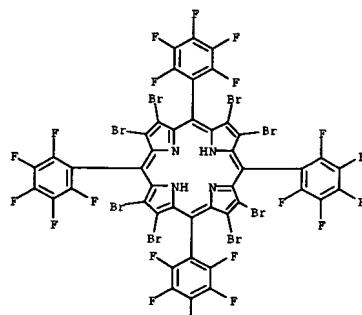


AB The invention relates to a recordable optical disk contains a novel polyolefin derivative represented by a general formula I (M = 2 hydrogen atoms, metal atom X1-8 = H, F, alkyl, alkoxy; R1-4 = alicyclic substituent) in recording layer. The recordable optical disk shows high sensitivity at a blue region.  
IT 129006-48-0 139944-26-6 161405-60-3  
RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)  
(polyolefin derivative in recordable optical disk suitable for readout at 400-450 nm)  
RN 129006-48-0 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

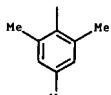
PAGE 1-A



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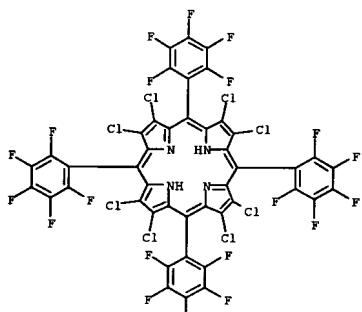
PAGE 2-A



RN 161405-60-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

RN 139944-26-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

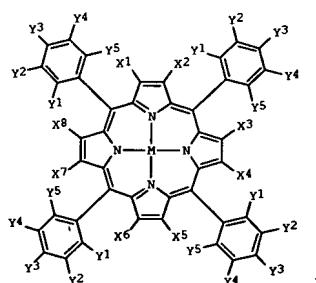
PAGE 1-A



16 ANSWER 44 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 2001:371489 CAPLUS  
 ACCESSION NUMBER: 134:359571  
 DOCUMENT NUMBER: Recordable optical disk suitable for readout at  
 400-450 nm  
 TITLE: Sasa, Noboru  
 INVENTOR(S): Ricoh Co., Ltd., Japan  
 PATENT ASSIGNEE(S): Jpn. Kokai Tokkyo Koho, 12 pp.  
 SOURCE: CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PARENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001138633	A2	20010522	JP 1999-322756	19991112
PRIORITY APPLN. INFO.:			JP 1999-322756	19991112
OTHER SOURCE(S):	MARPAT	134:359571		
GI				

PAGE 2-A



I

AB The invention relates to a recordable optical disk contains a novel polyolefin derivative represented by a general formula I (M = 2 hydrogen atoms, metal atoms; X1-8 = H, F; Y1-5 = H, halo, nitro, cyano, OH, carboxyl, alkyl, alkoxy, aryl, amino, acyl) in a recording layer. The recordable optical disk shows high sensitivity at a blue region.

IT 121399-88-0 129006-48-0 139944-26-6  
 161405-60-3 166885-28-9 339274-24-7

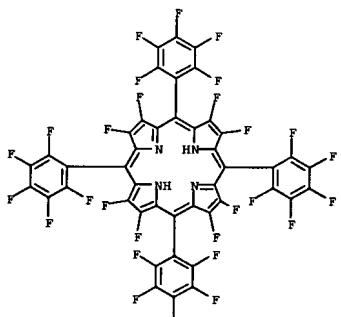
RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(polyolefin derivative in recordable optical disk suitable for readout at 400-450 nm)

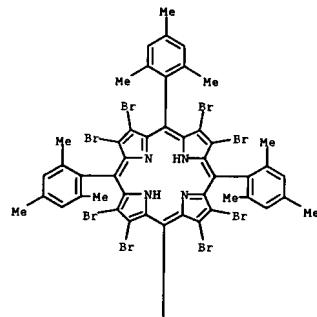
RN 121399-88-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafuoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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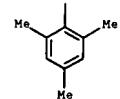


PAGE 2-A



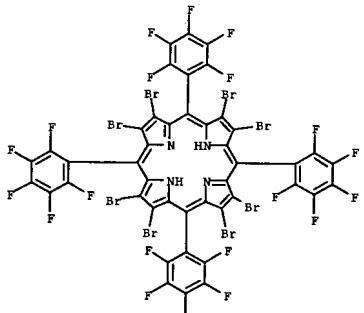
RN 129006-48-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

PAGE 2-A

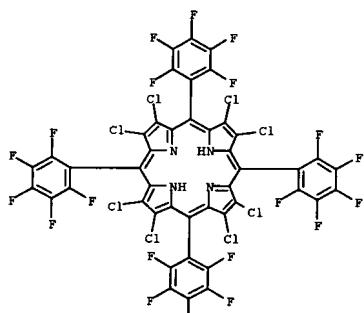


RN 139944-26-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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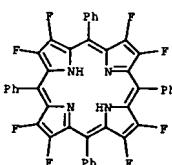


RN 161405-60-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

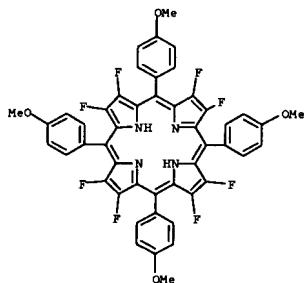
PAGE 2-A



RN 186885-28-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

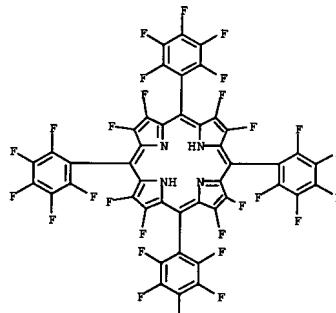


RN 339274-24-7 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 45 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 2001:294039 CAPLUS  
 135:83504  
 DOCUMENT NUMBER:  
 TITLE: Structure and Photophysics of  $\beta$ -Octafluoro-meso-tetraarylporphyrins  
 AUTHOR(S): Smirnov, Valeriy V.; Weller, Eric K.; Tatman, Derek; DiMaggio, Stephen G.  
 CORPORATE SOURCE: Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE, 68588-0304, USA  
 SOURCE: Inorganic Chemistry (2001), 40(11), 2614-2619  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The structure of THF-coordinated [2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenylporphyrinato]zinc, Zn(F8TPP)·THF, and photophysics studies of 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenylporphyrin, F8TPP, Zn(F8TPP), 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin, F28TPP, and [2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrinato]zinc, Zn(F28TPP), in benzonitrile, are reported. The octafluorinated F8TPP and perfluorinated F28TPP porphyrins possess similar absorption spectra, but dissimilar x-ray crystal structures and disparate photophysical characteristics. These data cannot be easily accommodated within currently accepted theories which relate macrocycle distortion and optoelectronic properties.  
 IT 121399-88-9 186885-28-9  
 RL: PRP (Properties)  
 (optical and photophys. properties)  
 RN 121399-88-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

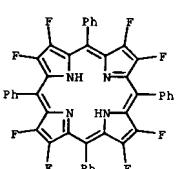
PAGE 1-A



PAGE 2-A

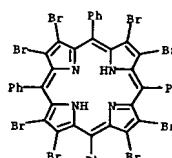
F

RN 186885-28-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 46 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 2001:85243 CAPLUS  
 134:320094  
 DOCUMENT NUMBER:  
 TITLE: Perbrominated 2-nitrotetraphenylporphyrins: electrochemical and axial ligation properties  
 AUTHOR(S): Bhryappa, Puttaiah; Purushothaman, Bhavana  
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology-Madras, Chennai, 600 036, India  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 2 (2001), (2), 238-242  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:320094  
 AB Perbrominated 2-nitro-5,10,15,20-tetraphenylporphyrins, H2TPPBn(NO2) (n = 6 and 7) and their metal (CuII and ZnII) complexes were synthesized and characterized. The presence of mixed electron withdrawing (bromo- and nitro-) substituents at the  $\beta$ -pyrrole positions induces interesting electrochem. and axial ligation properties. Perbrominated nitroporphyrins exhibit two successive one electron redox potentials with a pos. shift of >100 mV relative to their corresponding octabromotetraphenylporphyrin (MTPPB8) complexes. Axial ligation of various nitrogenous bases to ZnTPPBn(NO2) complexes showed facile ligand binding with >50% enhancement in the equilibrium consts., K<sub>eq</sub>, relative to ZnTPPB8. Surprisingly, H2TPPBn(NO2) complexes show similar axial ligation and electrochem. redox behavior. The anodic shift in electrochem. redox potentials and enhanced K<sub>eq</sub> of H2TPPBn(NO2) complexes were attributed to the increased electron deficiency of the porphyrin x-system.  
 IT 131214-86-3P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation, electronic spectrum and electrochem. redox, and complexation with copper and zinc)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2000:870724 CAPLUS

DOCUMENT NUMBER: 134:222261

TITLE: Oxidation of alkanes and alkenes by iodosylbenzenes and hydrogen peroxide catalyzed by halogenated manganese porphyrins in homogeneous solution and covalently bound to silica

AUTHOR(S): Doro, F. G.; Smith, J. R. L.; Ferreira, A. G.; Assis, M. D.

CORPORATE SOURCE: Departamento de Quimica, Universidade de Sao Paulo, Faculdade de Filosofia Ciencias e Letras de Ribeirao Preto, Ribeirao Preto, Sao Paulo, 14040-901, Brazil

SOURCE: Journal of Molecular Catalysis A: Chemical (2000), 164 (1-2), 97-108

CODEN: JMCAE2; ISSN: 1381-1169

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:222261

AB Manganese(III) 5-(pentafluorophenyl)-10,15,20-tri(2,6-dichlorophenyl)porphyrin, Mn(PFTDCPP), and manganese(II) 2,3,7,8,12,13,17,18-octachloro-5-(pentafluorophenyl)-10,15,20-tri(2,6-dichlorophenyl)porphyrin, Mn(PFTDC18PP), have been synthesized and used as catalysts in hydrocarbon oxidations, by iodosylbenzenes and hydrogen peroxide both in solution and covalently bound to aminopropylated silica. The former shows higher efficiency in the epoxidation of alkenes by iodosylbenzene, whereas the perchlorinated manganese porphyrin is more efficient in the hydroxylation of alkanes by this oxidant. The supported manganese(III) porphyrin show the same activity as its homogeneous analog. With hydrogen peroxide as oxygen donor, Mn(PFTDCPP) is a stable and effective catalyst in the presence of imidazole. The perchlorinated analog is a poor catalyst with this oxidant. The eight addnl. chlorine atoms on the porphyrin ring stabilize Mn(II) and unfavor the formation of the active species, MnV:O.

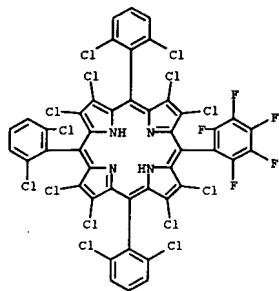
IT 328897-67-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(oxidation of alkanes and alkenes by iodosylbenzene and hydrogen peroxide catalyzed by halogenated manganese porphyrins in homogeneous solution and covalently bound to silica)

RN 328897-67-2 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15-tris(2,6-dichlorophenyl)-20-(pentafluorophenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

64

THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2000:802778 CAPLUS

DOCUMENT NUMBER: 134:100852

TITLE: Direct Synthesis of Expanded Fluorinated Calix[n]pyrroles: Decafluorocalix[5]pyrrole and Hexadecafluorocalix[9]pyrrole

AUTHOR(S): Sessler, Jonathan L.; Anzenbacher, Pavel, Jr.; Shriner, James A.; Jursikova, Karolina; Lynch, Vincent M.; Marquez, Manuel

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Journal of the American Chemical Society (2000), 122(48), 12061-12062

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:100852

AB Methanesulfonic acid-catalyzed condensation of 3,4-difluoropyrrole and acetone gives, in addition to octafluorocalix[4]pyrrole, the dominant reaction product, appreciable quantities of both the corresponding calix[5] and calix[9] products.

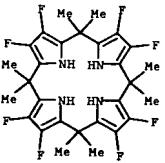
IT 311804-81-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of fluorinated calix[n]pyrroles)

RN 311804-81-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafuoro-5,10,15,20,22,24-hexahydro-5,6,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2000:735661 CAPLUS

DOCUMENT NUMBER: 134:91666

TITLE: Metalloporphyrin catalytic oxidations of hydrocarbons by H2O2

AUTHOR(S): Rocha Gonsalves, Antonio M. d'A.; Serra, Armenio C. Departamento de Quimica, Universidade de Coimbra, Coimbra, P-3049, Port.

CORPORATE SOURCE: Journal of Porphyrins and Phthalocyanines (2000), 4 (6), 598-603

SOURCE: CODEN: JPPHZ; ISSN: 1088-4246

PUBLISHER: John Wiley &amp; Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The metalloporphyrin catalytic oxidation of hydrocarbons using dilute hydrogen

peroxide as oxygen donor with a two-phase system in the presence of an excess of benzoic acid is studied. Porphyrins derived from meso-tetrakis(2,6-dichlorophenyl)porphyrin and bearing sulfonyl amide substituents at  $\beta$  or meso positions and halogens at  $\beta$  positions were used. The system allowed for very efficient catalytic epoxidations and hydroxylations of hydrocarbons. It is proved that the excess of benzoic acid is critical to the catalyst efficiency and stability. The role of the lipophilic acid in this system is discussed.

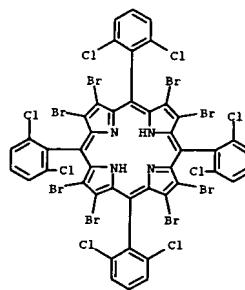
IT 107035-95-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(metalloporphyrin catalytic oxidns. of hydrocarbons by H2O2)

RN 107035-95-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

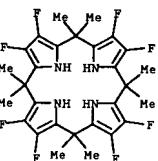
13

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 50 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2000:707590 CAPLUS  
 DOCUMENT NUMBER: 134:29395  
 TITLE: Fluorinated Calix[4]pyrrole and Dipyrrolylquinoxaline: Neutral Anion Receptors with Augmented Affinities and Enhanced Selectivities  
 AUTHOR(S): Anzenbacher, Pavel, Jr.; Try, Andrew C.; Miyaji, Hidekazu; Jursikova, Karolina; Lynch, Vincent M.; Marquez, Manuel; Sessler, Jonathan L.  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-1167, USA  
 SOURCE: Journal of the American Chemical Society (2000), 122(42), 10268-10272  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Octamethylcalix[4]pyrrole and 2,3-di(3,4-difluoropyrrol-2-yl)quinoxaline were prepared from 3,4-difluoropyrrole. These latter two entities act as neutral anion receptors and bind anions such as fluoride, chloride, or dihydrogen phosphate with an enhanced affinity compared to their non-fluorinated congeners as judged from <sup>1</sup>H NMR, <sup>19</sup>F NMR, and fluorescence emission spectroscopic analyses. The increase in affinity was especially high in case of chloride and dihydrogen phosphate anion, with the 2,3-di(3,4-difluoropyrrol-2-yl)quinoxaline system, in particular, displaying an affinity for H<sub>2</sub>PO<sub>4</sub><sup>-</sup> that was improved by 3 orders of magnitude as compared to its non-fluorinated congener. This improvement in the affinity for the dihydrogen phosphate is accompanied by change of color from pale yellow to orange, thus allowing the use of such compds. as naked-eye sensors for phosphate anion. In the case of the octafluorocalix[4]pyrrole system X-ray diffraction analyses revealed the presence of four different macrocyclic conformations in the solid state, as well as close intermol. contacts mediated by apparent CF<sub>3</sub>-HN hydrogen bonds.

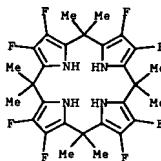
IT 311804-81-6P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and anion binding by octafluoroctamethylcalixpyrrole and bis(difluoropyrrolyl)quinoxaline)  
 RN 311804-81-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



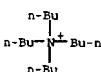
IT 311804-87-2P 311804-88-3P 311804-89-4P  
 311804-94-1P

L6 ANSWER 50 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and anion binding by octafluoroctamethylcalixpyrrole and bis(difluoropyrrolyl)quinoxaline)  
 RN 311804-87-2 CAPLUS  
 CN 1-Butanaminium, N,N,N-triethyl-, fluoride, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CH 1  
 CRN 311804-81-6  
 CMF C28 H28 F8 N4



CH 2  
 CRN 429-41-4  
 CMF C16 H36 N . F



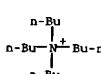
● F<sup>-</sup>  
 RN 311804-88-3 CAPLUS  
 CN 1-Butanaminium, N,N,N-triethyl-, chloride, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)  
 CH 1  
 CRN 311804-81-6  
 CMF C28 H28 F8 N4

L6 ANSWER 50 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 CRN 5574-97-0  
 CMF C16 H36 N . H2 O4 P

CH 3  
 CRN 14066-20-7  
 CMF H2 O4 P

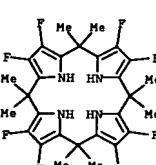


CH 4  
 CRN 10549-76-5  
 CMF C16 H36 N



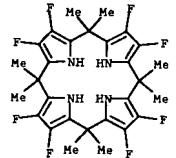
RN 311804-94-1 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-, compd. with sulfonylbis(methane) (1:1) (9CI) (CA INDEX NAME)

CH 1  
 CRN 311804-81-6  
 CMF C28 H28 F8 N4



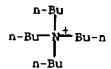
CH 2  
 CRN 67-68-5  
 CMF C2 H6 O S

L6 ANSWER 50 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CH 2

CRN 1112-67-0  
 CMF C16 H36 N . Cl .

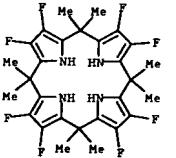


● Cl<sup>-</sup>

RN 311804-89-4 CAPLUS  
 CN 1-Butanaminium, N,N,N-triethyl-, phosphate, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 311804-81-6  
 CMF C28 H28 F8 N4



CH 2

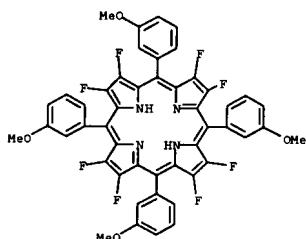
CRN 67-68-5  
 CMF C2 H6 O S



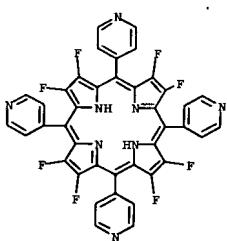
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 51 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2000:680398 CAPLUS  
 DOCUMENT NUMBER: 133:252219  
 TITLE: synthesis of octafluoro-meso-tetraarylporphyrins and their metal complexes for use as catalysts  
 INVENTOR(S): DiMaggio, Stephen G.  
 PATENT ASSIGNEE(S): University of Nebraska-Lincoln, USA  
 SOURCE: U.S., 10 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6124452	A	20000926	US 1997-994891	19971219
PRIORITY APPLN. INFO.: US 1997-994891 19971219				
OTHER SOURCE(S): CASREACT 133:252219; MARPAT 133:252219				
AB The title compds. are synthesized by reacting 3,4-difluoropyrrole with an aromatic aldehyde in the presence of boron trifluoride etherate, followed by oxidation. The difluoropyrrole used in this reaction is produced by reacting 3,3,4,4-tetrafluoropyrrolidine or its corresponding salt, 3,3,4,4-tetrafluoropyrrolidinium salt, with a base such as potassium tert-butoxide. The metalloporphyrins of the present invention are synthesized by deprotonating $\beta$ -octafluoro-meso-tetraarylporphyrin ligands and treating said ligands with metal ions.				
IT 186885-29-OP 295778-60-8P				
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (synthesis of octafluoro-meso-tetraarylporphyrins and their metal complexes for use as catalysts)				
RN 186885-29-0 CAPLUS				
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(3-methoxyphenyl)- (9CI) (CA INDEX NAME)				



RN 295778-60-8 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

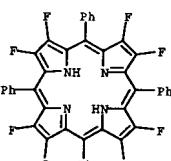


IT 121399-88-OP 186885-28-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PACT (Reactant or reagent)  
 (synthesis of octafluoro-meso-tetraarylporphyrins and their metal complexes for use as catalysts)  
 RN 121399-88-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

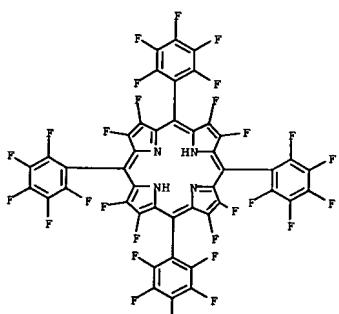
PAGE 2-A

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RN 186885-28-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



L6 ANSWER 52 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2000:570824 CAPLUS  
DOCUMENT NUMBER: 133:296117

TITLE: Umpolung of a Metal-Carbon Bond: A Potential Route to Porphyrin-Based Methane Functionalization Catalysts  
AUTHOR(S): Nelson, Andrew P.; DiMaggio, Stephen G.  
CORPORATE SOURCE: Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE, 68588-0304, USA  
SOURCE: Journal of the American Chemical Society (2000), 122(35), 8569-8570  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A modified Ru porphyrin complex performs each of the reactions in a formal catalytic cycle involved in converting methane, triphenylphosphine, and strong acid to a methylphosphonium salt and dihydrogen. The key design principle, that ligand modification can so increase metal nucleophilicity that nucleophilic substitution can be activated without compromising alkane and H activation, is drawn directly from fundamental concepts of chemical bonding. Developing an efficient catalytic system from these or similar components requires dramatically accelerated rates of the methane activation and nucleophilic functionalization.

IT 121399-88-0 CAPLUS  
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(ligands; umpolung of metal-carbon bond and route to porphyrin-based methane functionalization catalysts)

RN 121399-88-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

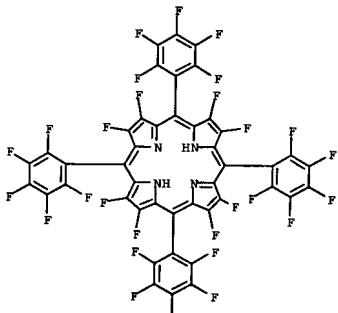
L6 ANSWER 52 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

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REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PAGE 1-A



L6 ANSWER 53 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2000:472188 CAPLUS  
DOCUMENT NUMBER: 133:202236

TITLE: Halogenation of metallocporphyrins  
AUTHOR(S): Rumyantseva, V. D.; Aksanova, E. A.; Ponamoreva, O. N.; Mironov, A. F.  
CORPORATE SOURCE: Lomonosov State Academy of Fine Chemical Technology, Moscow, 117571, Russia  
SOURCE: Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya) (2000), 26(6), 423-428  
CODEN: RJBCCF; ISSN: 1068-1620

PUBLISHER: MAI Nauka/Interperiodica

DOCUMENT TYPE: Journal

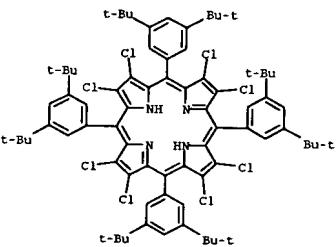
LANGUAGE: English

AB Thionyl chloride can chlorinate porphyrin complexes with transient metals (Pd, Ni, or Cu) at the free  $\beta$  and meso-positions of the porphyrin macrocycle. A more prolonged or rigorous treatment also causes the chlorination of side alkyl substituents, mainly, Me groups.

IT 288843-06-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation from chlorination of metallocporphyrins)

RN 288843-06-1 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20-tetrakis[3,5-bis(1,1-dimethylethyl)phenyl]-, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 54 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2000:426679 CAPLUS  
DOCUMENT NUMBER: 133:266543

TITLE: The oxidation of ethylbenzene and other alkylaromatics by dioxygen catalyzed by iron(III) tetrakis(pentafluorophenyl)porphyrin and related iron porphyrins

AUTHOR(S): Evans, Steven; Lindsay Smith, John R.  
CORPORATE SOURCE: Department of Chemistry, University of York, York, YO10 5DD, UK

SOURCE: Perkin 2 (2000), (7), 1541-1552

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:266543

AB The oxidation of ethylbenzene with dioxygen catalyzed by iron(III) porphyrins

in a solvent free system was studied over the temperature range 30-110

°C. The time dependence of the formation of the three main products, 1-phenylethanol, acetophenone and 1-phenylethyl hydroperoxide, and the fate of the iron porphyrin are interpreted in terms of a free radical autoxidn. mechanism. The yields of the oxidation products are determined

by the rate of reaction and by the lifetime of the catalyst. Catalyst degradation is shown to involve reaction of the porphyrin ligand with 1-phenylethoxyl and 1-phenylethylperoxy radicals. The disadvantages of increased induction periods and longer reaction times of the oxidants, observed

at lower reaction temps. are counter balanced by increased catalyst turnovers. Less extensive studies on the oxidants, of toluene, cumene, (2-methylpropyl)benzene and tert-butylbenzene support the overall mechanism proposed for ethylbenzene. A comparative study using the catalysts iron(III) 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)porphyrin and iron(III) tetrakis(pentafluorophenyl)porphyrin and five of its derivs. reveals that halogenation of the  $\beta$ -pyrrole positions markedly increases the activity of the catalysts but not the stability of the porphyrin towards degradation. The highest yields were obtained with the  $\mu$ -oxo dimer of iron(III) tetrakis(pentafluorophenyl)porphyrin and iron(III) tetrakis(4-dimethylamino-2,3,5,6-tetrafluorophenyl)porphyrin.

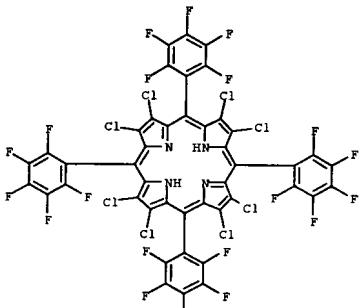
IT 161405-60-3P, 2,3,7,8,12,13,17,18-Octachloro-5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-Porphine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(oxidation of (alkyl)benzenes by dioxygen catalyzed by iron porphyrins)

RN 161405-60-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

16 ANSWER 55 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 2000:417208 CAPLUS  
 133:213839  
 TITLE: Mechanistic Studies of (Porphinato)Iron-Catalyzed Isobutane Oxidation. Comparative Studies of Three Classes of Electron-Deficient Porphyrin Catalysts

AUTHOR(S): Moore, Kevin T.; Horvath, Istvan T.; Therien, Michael J.  
 CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104-6323, USA  
 SOURCE: Inorganic Chemistry (2000), 39(15), 3125-3139  
 CODEN: IOCQJ ISSN: 0020-1669

PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

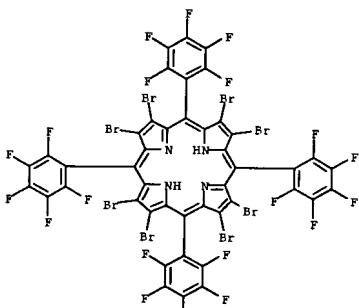
AB We report herein a comprehensive study of (porphinato)iron [PFe]-catalyzed isobutane oxidation in which mol. oxygen is utilized as the sole oxidant; these catalytic reactions were carried out and monitored in both autoclave reactors and sapphire NMR tubes. In situ <sup>19</sup>F and <sup>13</sup>C NMR expts., coupled with GC analyses and optical spectra obtained from the autoclave reactions have enabled the identification of the predominant porphyrin species present during PFe-catalyzed oxidation of isobutane. Electron-deficient PFe catalysts based on 5,10,15,20-tetrakis(pentafluorophenyl)porphyrin [(C6F5)<sub>4</sub>Fe]<sub>2</sub>, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin [Br<sub>8</sub>(C6F5)<sub>4</sub>Fe]<sub>2</sub>, and 5,10,15,20-tetrakis(heptafluoropropyl)porphyrin [(C3F<sub>7</sub>)<sub>4</sub>Fe]<sub>2</sub>] macrocycles were examined. The nature and distribution of hydrocarbon oxidation products show that an autoxid. reaction pathway dominated the reaction kinetics, consistent with a radical chain process. For each catalytic system examined, PFe<sup>II</sup> species were shown not to be stable under moderate O<sub>2</sub> pressure at 80 °C; in every case, the PFe<sup>II</sup> catalyst precursor was converted quant. to high-spin PFe<sup>III</sup> complexes prior to the observation of any hydrocarbon oxidation products. Once catalytic isobutane oxidation is initiated, all reactions are marked by concomitant decomposition of the porphyrin-based catalyst. In situ <sup>17</sup>O NMR spectroscopic studies confirm the incorporation of <sup>17</sup>O from labeled water into the oxidation products, implicating the involvement of PFe-OH in the catalytic cycle. Importantly, Br<sub>8</sub>(C6F<sub>5</sub>)<sub>4</sub>Fe-based catalysts, which lack macrocycle C-H bonds, do not exhibit augmented stability with respect to analogous catalysts based on (C6F<sub>5</sub>)<sub>4</sub>Fe and (C3F<sub>7</sub>)<sub>4</sub>Fe species. The data presented are consistent with a hydrocarbon oxidation process in which PFe complexes play dual roles of radical chain initiator, and the species responsible for the catalytic decomposition of organic peroxides. This modified Haber-Weiss reaction

scheme provides for the decomposition of tert-Bu hydroperoxide intermediates via reaction with PFe-OH complexes; the PFe<sup>III</sup> species responsible for hydroperoxide decomposition are regenerated by reaction of PFe<sup>II</sup> with dioxigen.

AB under these exptl. conditions.

IT 139944-26-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (studies of (porphinato)iron-catalyzed isobutane oxidation)  
 RN 139944-26-6 CAPLUS  
 CN 21H, Z3H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



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REFERENCE COUNT: 94 THERE ARE 94 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

16 ANSWER 56 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 2000:282110 CAPLUS  
 133:43367

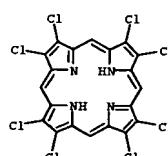
TITLE: Triplet Excited States of Free-Base Porphin and Its  $\beta$ -Octahalogenated Derivatives  
 AUTHOR(S): Nguyen, Kiet A.; Day, Paul N.; Pachter, Ruth  
 CORPORATE SOURCE: Air Force Research Laboratory, Materials and Manufacturing Directorate AFRL/MLPV, Wright-Patterson Air Force Base, OH, 45433-7702, USA  
 SOURCE: Journal of Physical Chemistry A (2000), 104(20), 4748-4754

PUBLISHER: JPCAPHA ISSN: 1089-5639  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

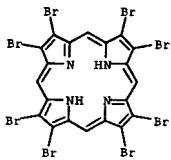
AB D. functional theory (DFT) electronic structure calcns. were carried out to predict the structures, energetics, and triplet-triplet (T-T) spectra for the low-lying triplet states of free-base porphin (PH2) and its  $\beta$ -octahalogenated derivs. ( $\beta$ -PH2X<sub>8</sub>; X = F, Cl, Br). The lowest triplet excited state of PH2 and  $\beta$ -PH2X<sub>8</sub> was found to retain D<sub>2h</sub> symmetry with stretched C<sub>B</sub>-C<sub>H</sub> and C<sub>B</sub>-C<sub>m</sub> bond distances. For free-base porphin, the singlet-triplet (S<sub>0</sub>-T<sub>1</sub>) gap obtained with the B3LYP functional was in excellent agreement with the exptl. phosphorescence value. Excitation energies computed by time-dependent DFT also provided a fine account of the observed T-T spectrum.  $\beta$ -Halogenation had little effect on the singlet-triplet gaps of porphin. The S<sub>0</sub>-T<sub>1</sub> and S<sub>0</sub>-T<sub>2</sub> splittings for  $\beta$ -PH2X<sub>8</sub> were within 0.1 eV of the corresponding splittings in the unsubstituted porphin. All bands in the T-T spectra of  $\beta$ -PH2X<sub>8</sub> were predicted to be significantly (up to 0.65 eV) red-shifted in comparison to corresponding bands of the unsubstituted porphin.

IT 144811-81-6, Octachloroporphine 144811-86-9, Octafluoroporphine  
 RL: PRP (Properties)  
 (triplet excited states of free-base porphine and its  $\beta$ -octahalogenated derivs.)

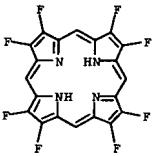
RN 144811-81-4 CAPLUS  
 CN 21H, Z3H-Porphine, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)



RN 144811-83-6 CAPLUS  
 CN 21H, Z3H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



RN 144811-86-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)



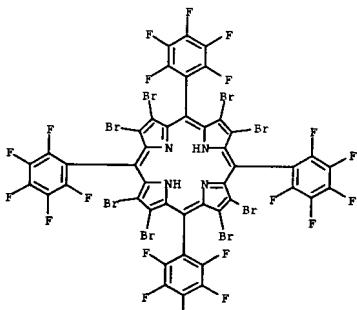
REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 57 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999;770768 CAPLUS  
 DOCUMENT NUMBER: 132:129866  
 TITLE: Photocatalytic activation of oxygen by iron(III) porphyrins  
 AUTHOR(S): Hennig, Horst; Lappa, Doritt  
 CORPORATE SOURCE: Institut fur Anorganische Chemie, Universitat Leipzig, Leipzig, D-04103, Germany  
 SOURCE: Journal fuer Praktische Chemie (Weinheim, Germany) (1999), 341(8), 757-767  
 CODEN: JCCHF4; ISSN: 1436-9966  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German

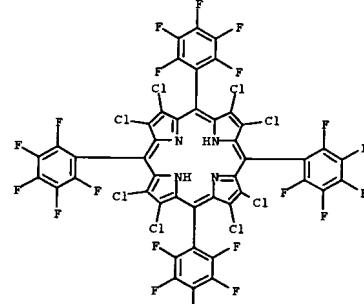
AB Photoc. charge transfer excitation of tetraphenyl(porphyrinato)iron(III) complexes yields tetraphenyl(porphyrinato)iron(II) which is able to coordinate O<sub>2</sub> under formation of oxo-[tetraphenyl(porphyrinato)iron(IV)]. Based on this photochem. reaction pathway photocatalytic oxygenation of  $\alpha$ -pinene and other alkenes can be initiated. Fe(III) complexes of tetramesitylporphyrin, tetrakis(pentafluorophenyl)porphyrin, octa- $\beta$ -bromo-tetrakis(pentafluorophenyl)porphyrin, and octa- $\beta$ -chloro-tetrakis(pentafluorophenyl)porphyrin were investigated photochem. with the aim to improve the low photochem. efficiency of tetraphenyl(porphyrinato)iron(III). The influence of substituents on the porphyrin ligand on the photochem. behavior of the corresponding Fe(III) complexes is measured mainly by temperature dependent UV/Vis spectroscopy. Both, the yield of oxygenation products formed photocatalytically with  $\alpha$ -pinene and the product distribution (allylic alcs. vs. epoxide) depend on the design of the porphyrin ligands coordinated with Fe(III).  
 IT 139944-26-6 161405-60-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of Fe(III) porphyrin complexes)

RN 139944-26-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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RN 161405-60-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

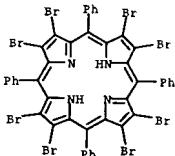
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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PAGE 2-A

16 ANSWER 58 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:770348 CAPLUS  
 DOCUMENT NUMBER: 132:92953  
 TITLE: Electronic effects on the stereoselectivity of epoxidation reactions catalyzed by manganese porphyrins  
 AUTHOR(S): Bacicocchi, Enrico; Boschi, Tristano; Cassioli, Luigi;  
 Galli, Carlo; Jaquinod, Laurent; Lapi, Andrea;  
 Paolese, Roberto; Smith, Kevin M.; Tagliatesta,  
 Pietro  
 CORPORATE SOURCE: Dipartimento Chimica, Univ. La Sapienza, Rome,  
 I-00185, Italy  
 SOURCE: European Journal of Organic Chemistry (1999), (12),  
 3281-3286  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A series of Mn(III) porphyrins progressively halogenated in the  $\beta$ -pyrrolic positions was employed to catalyze the epoxidation of cis-stilbene by iodosylbenzene, and to study the role of the electronic effects on the stereoselectivity of this process. A gradual improvement in the stereoselectivity on increasing the number of  $\beta$ -halogen atoms was observed. The role of steric effects upon the epoxidin, was also investigated by placing ortho-substituents in the meso- $\beta$  rings, and it was found that steric effects are more important than electronic effects toward the stereoselectivity of this process. These results can be rationalized by proposing a competition between a non-stereoselective electrophilic pathway of addition and a stereospecific pathway of O insertion, the former being disfavored by electron-withdrawing substituents. Alternatively, the formation of an open intermediate between the Mn(V) oxene and the substrate could be suggested, where the stereoselectivity ought to be determined by the competition between closure of the epoxide ring and rotation around the C-C bond. In this case, the enhanced stereoselectivity given by our polyhalogenated porphyrins might be attributed to an acceleration of the epoxide ring closure caused by the electron-withdrawing effect of the halogen substituents.  
 IT 131214-86-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (coordination) steric and electronic substituent effects of porphyrin ligands on Mn porphyrin-catalyzed stereoselective epoxidin. of cis-stilbene)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-  
 (9Cl) (CA INDEX NAME)



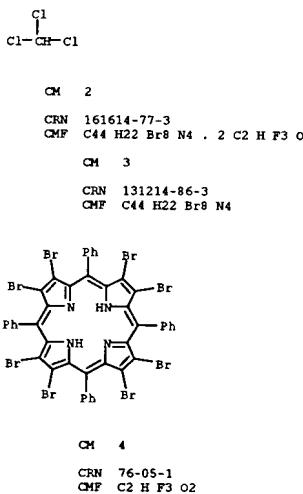
16 ANSWER 59 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999-529518 CAPLUS  
 DOCUMENT NUMBER: 131:351141  
 TITLE: Structure and conformation of tetra-meso-,  
 octa- $\beta$ -, and dodeca-substituted  
 22,24-dihydroporphyrins (porphyrin dications)  
 AUTHOR(S): Serge, Mathias O.; Kalisch, Werner W.  
 CORPORATE SOURCE: Institut Chemie, Organische Chemie, Freie Univ.  
 Berlin, Berlin, D-14195, Germany  
 SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences  
 (1999) 54 (7), 943-959  
 CODEN: ZNBSEN; ISSN: 0932-0776  
 PUBLISHER: Verlag der Zeitschrift fuer Naturforschung  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A comparative crystallographic anal of the conformation of porphyrin dicacids with various substituent types reveals considerable differences in the degree of nonplanarity and distortion modes. Dicacids of 5,10,15,20-tetraphenylporphyrins generally exhibit typical saddle-distorted macrocycles with displacements of the Cb positions in the range of 0.7-1.0 Å. Adding peripheral substituents, i.e., using dodeca-substituted porphyrins for the dicacid formation yields similar distortion types albeit with larger out-of-plane displacements. As a result of the combined effect of both peripheral (interaction between the Cb and Cm substituents) and core (interaction between the 4 inner H atoms) steric strain the maximum Cb displacements reach 1.3-1.5 Å. Quite a different situation is observed for the dicacids of 2,3,7,8,12,13,17,18-octaethylporphyrins. Here, macrocycles with pair-wise displacement of neighboring pyrrole rings and significant NH pyramidalization and those with classic saddle distortion are found. Generally, octa- $\beta$ -substituted porphyrin dicacids show smaller degrees of nonplanarity: Cb displacements ranged from 0.6 to 0.72 Å. On the basis of the overall degree of conformational distortion ( $A_{24}$  = average deviation of the 24 macrocycles atoms from the mean plane), the 3 different types of porphyrin macrocycles studied differ considerably in their degree of conformational flexibility. For several porphyrin crystal structures with different counterions and/or solvate mol<sup>-1</sup> were obtained. Taking into account results from the literature, 2,3,7,8,12,13,17,18-octaethyl-22,24-dihydro-5,10,15,20-tetraphenylporphyrin shows the smallest degree of flexibility ( $A_{24}$  = 0.61-0.63 Å; 4 different x-ray structures), while 22,24-dihydro-5,10,15,20-tetraphenylporphyrin is more flexible ( $A_{24}$  = 0.42-0.52 Å; 4 structures). The largest flexibility is observed for 2,3,7,8,12,13,18-octaethyl-22,24-dihydroporphyrin ( $A_{24}$  = 0.02-0.33 Å; 4 structures).

IT 161614-78-4  
RL: PRP (Properties)  
(crystal structure)  
RN 161614-78-4 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,13,20-tetraphenyl-,  
bis(trifluoroacetate), compd. with trichloromethane (2:1) (9CI) [CA INDEX  
NAME]

CH 1

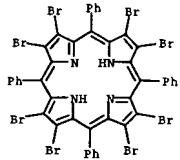
CRN 67-66-3  
QMP C H C13

L6 ANSWER 58 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



IT 161614-77-3P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (crystal structure and conformation of porphyrin dications)  
 RN 161614-77-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,13,20-tetraphenyl-  
 bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CH



CM 2

CRN 76-05-1  
CMF C2 H F3 O2

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1999:25327 CAPLUS

DOCUMENT NUMBER: 131:329692

TITLE: Intramolecular Electron Transfer of Diporphyrins Comprised of Electron-Deficient Porphyrin and Electron-Rich Porphyrin with Photocontrolled Isomerization. [Erratum to document cited in CA130:160405]

AUTHOR(S): Tsuchiya, Shinji

CORPORATE SOURCE: Institute Industrial Science, Univ. Tokyo, Tokyo, 106, Japan

SOURCE: Journal of the American Chemical Society (1999), 121(35), 8132

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB: The first two sentences in Reference 41 on page 6521 should be the following:

"(41) the syntheses of  $\beta$ -octafluorinated porphyrins using 3,4-difluoropyrrole as a precursor have been reported by DiMaggio and Lloyd. The compds. obtained from the 3,4-difluoropyrrole route have different phys. properties than those reported in reference 7 of J. Am. Chemical Society 1999, 121, 48-53."

IT 220213-35-4

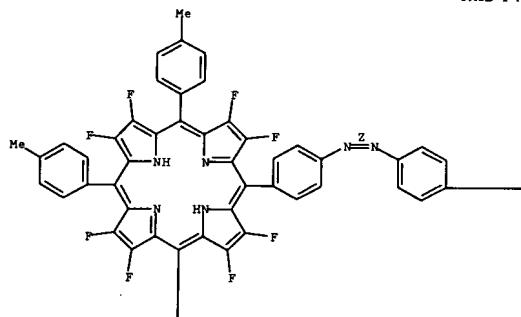
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)

RN 220213-35-4 CAPLUS

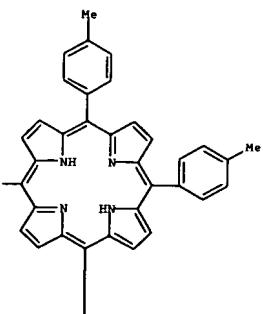
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-[4-[(12)-4-[10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-ylphenyl]azolphenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

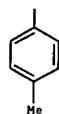
PAGE 1-A



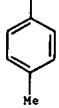
PAGE 1-B



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IT 220213-34-3P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(fluorescence and photoisomerization and photoinduced intramol.

electron-transfer of azobenzene-linked diporphyrin Zn complexes and

free base analogs (Erratum) (Erratum)

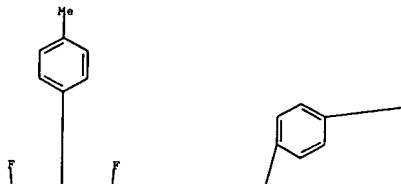
RN 220213-34-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-

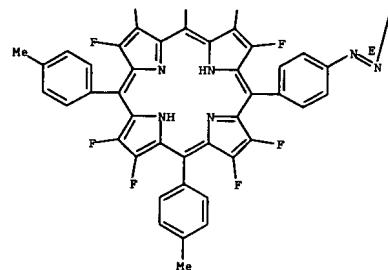
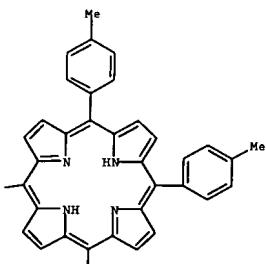
methylphenyl)-20-[4-[(1E)-4-[10,15,20-tris(4-methylphenyl)-21H,23H-

porphin-5-ylphenyl]azolphenyl]- (9CI) (CA INDEX NAME)

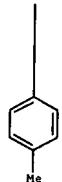
Double bond geometry as shown.



PAGE 1-B

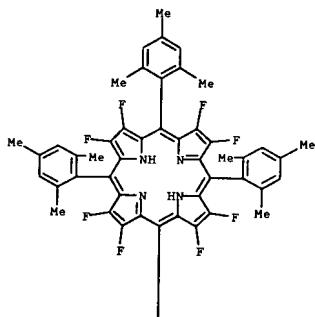


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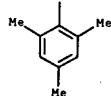


IT 220213-36-5  
 RL: PRP (Properties)  
 (fluorescence quenching by electron transfer from electron-rich to  
 electron-deficient porphyrin in relation to photophysics of  
 azobenzene-linked diporphyrins (Erratum) (Erratum))  
 RN 220213-36-5 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(2,4,6-  
 trimethylphenyl)- (9CI) (CA INDEX NAME)

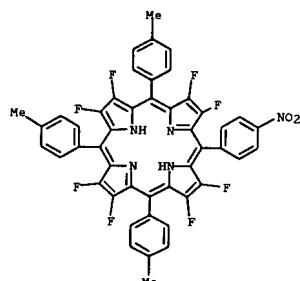
PAGE 1-A



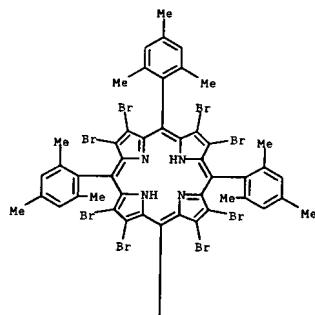
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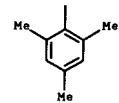
IT 220213-37-6  
 RL: FNU (Formation, unclassified); FORM (Formation, nonpreparative)  
 (in synthesis of azobenzene-linked diporphyrin Zn complexes (Erratum)  
 (Erratum))  
 RN 220213-37-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-  
 methylphenyl)-20-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 61 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:523271 CAPLUS  
 DOCUMENT NUMBER: 131:299306  
 TITLE: Novel dodecaarylporphyrins: synthesis and dynamic properties  
 AUTHOR(S): Muzzi, Cinzia M.; Medforth, Craig J.; Voss, Lisa; Cancilla, Mark; Lebrilla, Carlito; Ma, Jian-Guo; Shelnutt, John A.; Smith, Kevin M.  
 CORPORATE SOURCE: Department of Chemistry, University of California, Davis, CA, 95616, USA  
 SOURCE: Tetrahedron Letters (1999), 40(34), 6159-6162  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 131:299306  
 AB An investigation of the synthesis of dodecaarylporphyrins using the Suzuki coupling reaction of arylboronic acids with octabromotetraarylporphyrins is reported. Variable temperature <sup>1</sup>H NMR studies of these new porphyrins reveal several dynamic processes including the 1st examples of  $\beta$ -aryl rotation.  
 IT 129006-48-0 131214-86-3 139944-26-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactant for preparation of dodecaarylporphyrins)  
 RN 129006-48-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



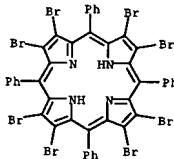
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L6 ANSWER 61 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

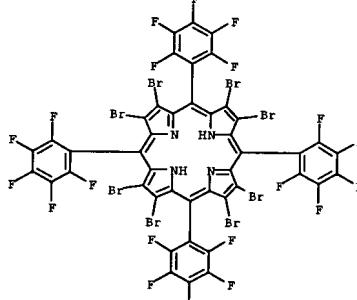
PAGE 2-A

RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



RN 139944-26-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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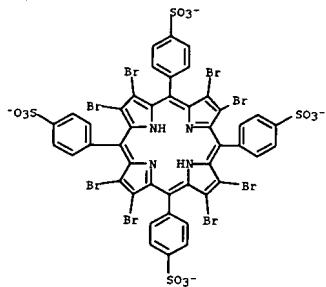
L6 ANSWER 61 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 62 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:416534 CAPLUS  
 DOCUMENT NUMBER: 131:96507  
 TITLE: Separation and transport of lithium of 10-5 M in the presence of sodium chloride higher than 0.1 M by 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin  
 AUTHOR(S): Sun, Haiping; Tabata, Masaki  
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840-8502, Japan  
 SOURCE: Talanta (1999), 49(3), 603-610  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A water-soluble porphyrin (2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin (H<sub>2</sub>(obtpps)<sub>4</sub><sup>-</sup>, H<sub>2</sub>P<sub>4</sub><sup>-</sup>)) synthesized in the laboratory was applied to a solvent extraction method and a liquid membrane transport of lithium  $\geq$ 10-5 M (M = mol dm<sup>-3</sup>) in the presence of sodium chloride >0.1 M. The lithium porphyrin with five neg. charges was extracted successfully into chloroform with tetrabutylammonium ion (Me<sub>3</sub>C)<sub>4</sub>N<sup>+</sup>) at pH 12.7. The extraction constant for the reaction of [LiP<sub>5</sub>]<sup>-</sup> + 5[(Me<sub>3</sub>C)<sub>4</sub>N]<sup>+</sup> .dblrw. [(Me<sub>3</sub>C)<sub>4</sub>N]<sup>5+</sup>P<sub>0</sub>] is  $(1.9 \pm 0.3) \times 10^{18}$  M<sup>-5</sup>, where the subscripts a and o denote chemical species in aqueous and organic phases, resp. Lithium was transported to an aqueous phase at pH 7 through a chloroform liquid membrane containing [(Me<sub>3</sub>C)<sub>4</sub>N]<sup>5+</sup>P<sub>0</sub>. The extraction and transport mechanism was discussed from extraction const., chemical species and transportation rate. Lithium in sea water or serum sample was separated and its concentration was determined spectrophotometrically by the present method without any interference from sodium chloride. The interference from transition and heavy metal ions was masked by Mg-EDTA. A calibration curve was linear at  $2 \pm 10^{-6}$  2 + 10-5 M at a precision of 1.5% (relative standard deviation).  
 IT 176173-80-1, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (lithium determination in sea water and serum by solvent extraction and spectrophotometry using octabromo tetrakis sulfonatophenyl porphyrin)  
 RN 176173-80-1 CAPLUS  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis-, ion(4-) (9CI) (CA INDEX NAME)

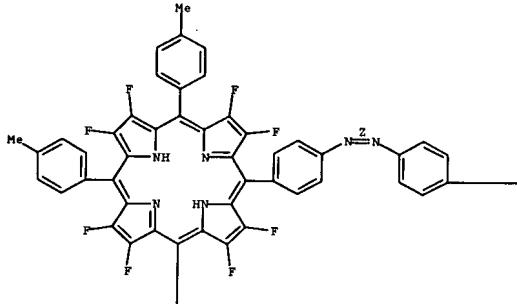


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

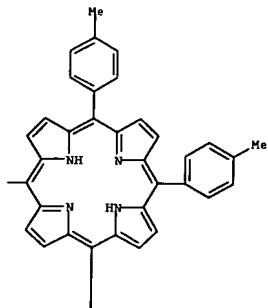
L6 ANSWER 63 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:395187 CAPLUS  
 DOCUMENT NUMBER: 131:235638  
 TITLE: Intramolecular Electron Transfer of Diporphyrins Comprised of Electron-Deficient Porphyrin and Electron-Rich Porphyrin with Photocontrolled Isomerization. [Erratum to document cited in CA130:160405]  
 AUTHOR(S): Tsuchiya, Shinji  
 CORPORATE SOURCE: Institute Industrial Science, Univ. Tokyo, Tokyo, 106, Japan  
 SOURCE: Journal of the American Chemical Society (1999), 121(27), 6521  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Reference 40 and 41 relevant to the work reported on page 53 are given.  
 IT 220213-35-4  
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)  
 (fluorescence and photoisomerization and photoinduced intramol. electron-transfer of azobenzene-linked diporphyrin Zn complexes and free base analogs (Erratum))  
 RN 220213-35-4 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-[4-[(1E)-[4-[10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-yl]phenyl]azophenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

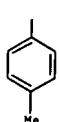
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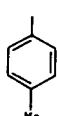
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IT 220213-34-3P  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
 (fluorescence and photoisomerization and photoinduced intramol. electron-transfer of azobenzene-linked diporphyrin Zn complexes and free base analogs (Erratum))  
 RN 220213-34-3 CAPLUS

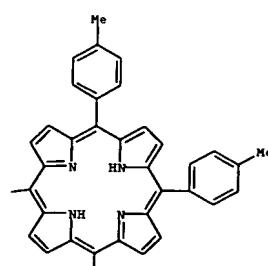
L6 ANSWER 63 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-[4-[(1E)-[4-[10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-yl]phenyl]azophenyl]- (9CI) (CA INDEX NAME)

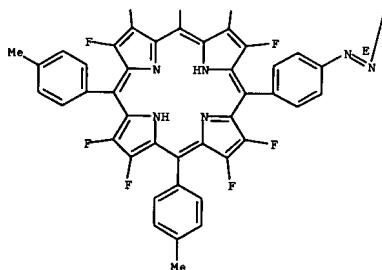
Double bond geometry as shown.

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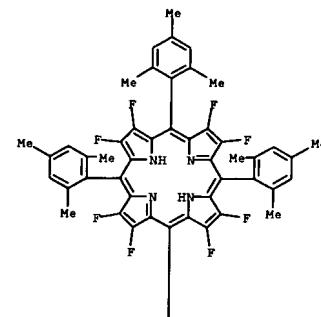


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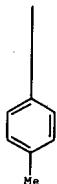




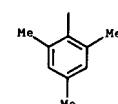
PAGE 2-A



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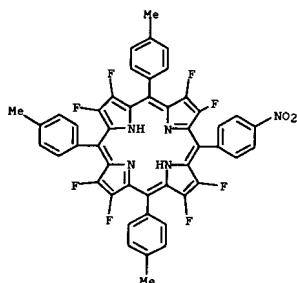
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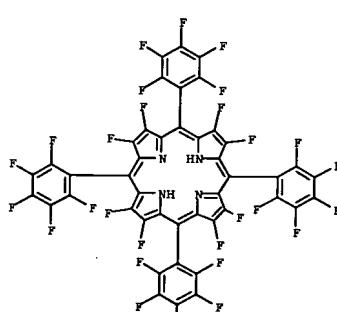
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IT 220213-36-5  
 RL: PRP (Properties)  
 (fluorescence quenching by electron transfer from electron-rich to electron-deficient porphyrin in relation to photophysics of azobenzene-linked diporphyrins (Erratum))  
 RN 220213-36-5 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

IT 220213-37-6  
 RL: PRM (Formation, unclassified); FORM (Formation, nonpreparative)  
 (in synthesis of azobenzene-linked diporphyrin Zn complexes (Erratum))  
 RN 220213-37-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



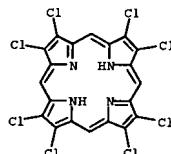
L6 ANSWER 64 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:269042 CAPLUS  
 DOCUMENT NUMBER: 130:304300  
 TITLE: 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin  
 AUTHOR(S): Leroy, Jacques; Bondon, Arnaud; Toupet, Loic  
 CORPORATE SOURCE: Ecole Normale Supérieure, Dep. Chim., URA CNRS, Paris, 75231, Fr.  
 SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (1999), C55(3), 464-466  
 PUBLISHER: Munksgaard International Publishers Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The core of the title compound, C44H2F28N4, is essentially planar while the pentafluorophenyl groups are nearly perpendicular to the mean porphyrin plane. The mol. is centrosym. Crystallog. data are given.  
 IT 121399-88-0  
 RL: PRP (Properties)  
 (crystal structure of)  
 RN 121399-88-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)



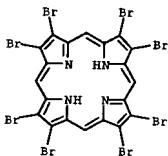
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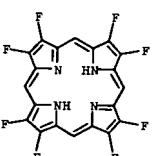
L6 ANSWER 65 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:260115 CAPLUS  
 DOCUMENT NUMBER: 131:129798  
 TITLE: Effects of halogenation on the ionized and excited states of free-base and zinc porphyrins  
 AUTHOR(S): Nguyen, Kiet A.; Day, Paul N.; Pachter, Ruth  
 CORPORATE SOURCE: Air Force Research Laboratory, AFRL/MLPJ, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH, 45433-7702, USA  
 SOURCE: Journal of Chemical Physics (1999), 110(18), 9135-9144  
 CODEN: JCPSA6; ISSN: 0021-9606  
 PUBLISHER: American Institute of Physics  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Ab initio electronic structure theory has been applied to study the effects of  $\beta$ -halogenation on the structure, ionization potentials (IP), and electronic spectra of free-base (Ph2) and zinc porphyrins (ZnPh). Electronic and IR (IR) spectra of  $\beta$ -octahalogenated free-base ( $\beta$ -ZnPhX8; X=F, Cl, Br) and zinc porphyrins ( $\beta$ -ZnFX8; X=F, Cl, Br) are predicted using TD-DFT, B3LYP, and CIS methods. Computations of the excitation energies and IP's are also carried out using structures obtained with the B3LYP d<sub>0</sub> functional. Valence IP's of Ph2 and ZnPh increase significantly upon  $\beta$ -halogenation. Except for the fluoro group, all  $\beta$ -halogen auxochromes slightly red shift the UV and visible bands of the free-base and zinc porphyrin chromophores.  $\beta$ -Halogenation significantly red shifts the B bands with increasing magnitude upon going down the period. In addition, we gauge the effects of  $\beta$ -halogenation on the thermodynamic stability of ZnPh by calculating the metal binding energies for  $\beta$ -ZnPhX8. The authors found that all  $\beta$ -ZnPhX8 have lower metal binding energies than the corresponding binding energy predicted for ZnPh. The metal binding energies for zinc porphyrins are significantly larger (apprx. 2 eV) than the H<sub>2</sub> elimination enthalpies of the corresponding free-base analogs.  
 IT 144811-81-4, Octachloroporphine 144811-83-6, Octabromoporphine 144811-86-9, Octafluoroporphine  
 RL: PRP (Properties)  
 (Effects of halogenation on the ionized and excited states of free-base and zinc porphyrins)  
 RN 144811-81-4 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)



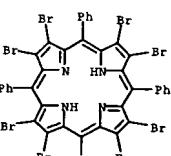
RN 144811-83-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



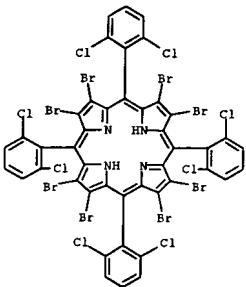
RN 144811-86-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)



L6 ANSWER 66 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:83211 CAPLUS  
 DOCUMENT NUMBER: 130:204223  
 TITLE: Synthesis and characterization of porphyrin complexes of iron(III) and manganese(III)  
 AUTHOR(S): Krishna, V.; Agarwal, D. D.; Bayrappa, G.; Rastogi, Rachana  
 CORPORATE SOURCE: Dept. of IPC, Indian Institute of Science, Bangalore, 560 012, India  
 SOURCE: Indian Journal of Chemistry, Section A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical Chemistry (1998), 37A(10), 918-920  
 CODEN: ICACEC; ISSN: 0376-4710  
 PUBLISHER: National Institute of Science Communication, CSIR  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The porphyrin complexes of Fe(III) and Mn(III) bearing electron withdrawing substituents at  $\beta$ -pyrrole carbons exhibit interesting electronic structure. Porphyrin ligands studied include 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-21H,23H-porphyrin and the 5,10,15,20-tetrakis(2,6-dichlorophenyl) derivative. The complexes are electroreactive and show reversible redox behavior. Coulometric data suggest that oxidation and reduction involves one-electron transfer each.  
 IT 131214-86-3  
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (complexation with iron(III) and manganese(III), and redox potentials of)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



IT 107035-95-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and complexation with iron(III) and manganese(III))  
 RN 107035-95-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

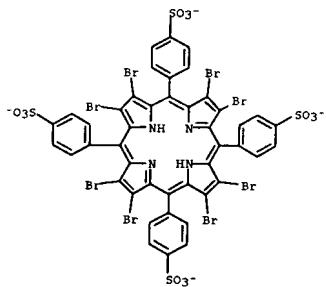


REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

16 ANSWER 67 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1999:19120 CAPLUS  
 DOCUMENT NUMBER: 130:162452  
 TITLE: Trace analysis of lithium with a water-soluble porphyrin  
 AUTHOR(S): Tabata, Masasaki; Sun, Haiping; Nishimoto, Jun  
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840-8502, Japan  
 SOURCE: Journal of Inclusion Phenomena and Molecular Recognition in Chemistry (1998), 32(2-3), 267-281  
 PUBLISHER: Kluwer Academic Publishers  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A water-soluble porphyrin (2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonophenyl)porphyrin; H<sub>2</sub>obtppp4-; H2P4-) was synthesized and developed for the determination and separation of Li<sup>+</sup> ion in aqueous solution. The octabromo groups lower the basicity of the porphyrin by their electron-withdrawing effect, and enable the porphyrin to react with Li<sup>+</sup> ion in alkaline aqueous solution to form the Li complex along with a shift of absorption maxima;  $\lambda_{max}$  (log  $\epsilon$ /mol<sup>-1</sup> dm<sup>3</sup> cm<sup>-1</sup>) of the Li porphyrin are 490.5 nm (5.31) and 734 nm (4.36). Na<sup>+</sup> and K<sup>+</sup> ions did not react with the porphyrin. The equilibrium constant for the reaction Li<sup>+</sup> + H<sub>2</sub>P4-  $\rightleftharpoons$  [LiP4-] is 10.8-79 and the conditional formation constant of the [LiP4-] at pH 13 is 104.21. The [LiP4-] can be extracted into CHCl<sub>3</sub> as an ion-pair complex with Bu<sub>4</sub>N<sup>+</sup> ion (X<sup>+</sup>) and the extracted X5LiP<sup>-</sup> dissociates to X4LiP<sup>-</sup> and X<sup>+</sup> in CHCl<sub>3</sub>. The extraction constant for the reaction of [LiP4-]a + 5[X<sup>+</sup>]a  $\rightleftharpoons$  [X4LiP<sup>-</sup>]a + [X<sup>+</sup>]a + 1012 mol<sup>-4</sup> dm<sup>12</sup>, where subscripts of a and o denote chemical species in aqueous and organic phases, resp. The above results were developed for the determination of Li in serum, sea water and hot spring H<sub>2</sub>O samples at 0.07-0.7 mg dm<sup>-3</sup> (1 + 10<sup>-5</sup> -1 + 10<sup>-4</sup> mol dm<sup>-3</sup>). The interference of heavy metal ions was masked by N,N'-1,2-ethanediylibis[N-(carboxymethyl)glycinate]magnesium(II) ([Mg(EDTA)]<sup>2-</sup>) or H<sub>4</sub>EDTA if sample contain Mg(II) ion.

IT 176173-80-1P, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetrakis(4-sulfonophenyl)porphyrin  
 RL: ARG (Analytical reagent use); PRP (Properties); SPP (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses) (trace determination of lithium with a water-soluble porphyrin by extraction-spectrophotometry)  
 RN 176173-80-1 CAPLUS  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis-, ion(4-) (9CI) (CA INDEX NAME)



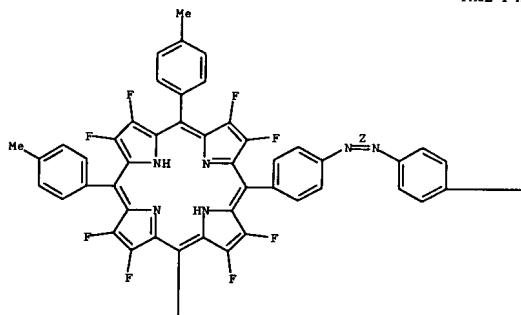
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

16 ANSWER 68 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1998:007525 CAPLUS  
 DOCUMENT NUMBER: 130:160405  
 TITLE: Intramolecular Electron Transfer of Diporphyrins Comprised of Electron-Deficient Porphyrin and Electron-Rich Porphyrin with Photocontrolled Isomerization  
 AUTHOR(S): Tsuchiya, Shinji  
 CORPORATE SOURCE: Institute of Industrial Science, University of Tokyo, Minato-Ku Tokyo, 106, Japan  
 SOURCE: Journal of the American Chemical Society (1999), 121(1), 48-53  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB New azobenzene-linked diporphyrin Zn complexes and free base analogs were synthesized in an attempt to develop new materials for mol. electronics. These diporphyrin Zn complexes and the corresponding diporphyrins consist of electron-deficient porphyrin Zn complex and electron-rich porphyrin Zn complex or electron-deficient porphyrin and electron-rich porphyrin. These compds., which are a new family of diporphyrins, exhibited the photoresponsive property with a structural change in the antenna; the trans-cis photoisomerization and cis-trans thermal recovery occurred and this process was reversible. A particularly noteworthy characteristic of the diporphyrin Zn complex is that its fluorescence spectrum changes with isomerization; the fluorescence intensity of the cis-isomer produced by photoirradn. is smaller than that of the trans-isomer. This fluorescence quenching of the cis-isomer arises from the intramol. electron transfer from electron-rich porphyrin Zn complex to electron-deficient porphyrin Zn complex. Similar phenomena were observed for azobenzene-linked diporphyrins. This discovery that intramol. electron transfer between the porphyrin rings is caused by photocontrolled isomerization is worthy of notice. Addnl., these compds. bearing eight fluorine atoms at the  $\beta$ -position of one porphyrin ring are the ideal materials for the practical application, because of their robust properties. This finding clearly suggests that new mol. are particularly useful in the development of photocontrolled mol. electronics such as mol. switches.

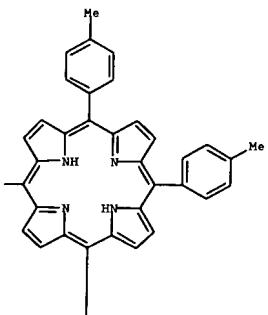
IT 220213-35-4  
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process) (fluorescence and photoisomerization and photoinduced intramol. electron-transfer of azobenzene-linked diporphyrin Zn complexes and free base analogs)  
 RN 220213-35-4 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-[4-((12)-[4-(10,15,20-tris(4-methylphenyl)-21H,23H-porphine-5-yl)phenyl]azo)phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

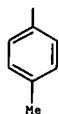
PAGE 1-A



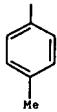
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IT 220213-34-3P

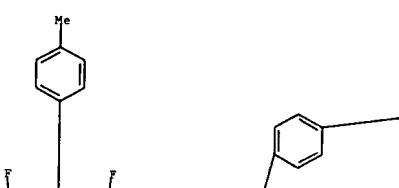
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (fluorescence and photoisomerization and photoinduced intramol. electron-transfer of azobenzene-linked diporphyrin Zn complexes and free base analogs)

RN 220213-34-3 CAPLUS

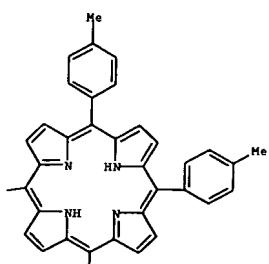
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-(4-[(1E)-{4-[10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-yl]phenyl}azolphenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

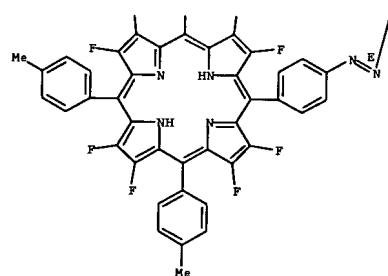
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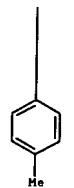
PAGE 1-B



PAGE 2-A



PAGE 2-B



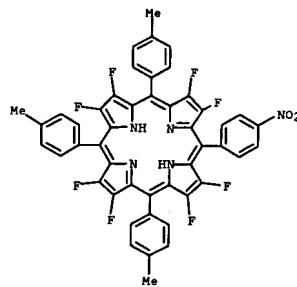
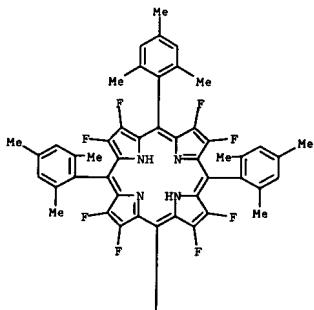
IT 220213-36-5

RL: PRP (Properties) (fluorescence quenching by electron transfer from electron-rich to electron-deficient porphyrin in relation to photophysics of azobenzene-linked diporphyrins)

RN 220213-36-5 CAPLUS

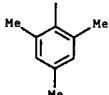
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

## PAGE 1-A



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

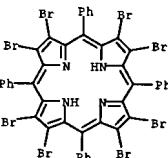
## PAGE 2-A



- IT 220213-37-6  
 RL: FNU (Formation, unclassified); FORM (Formation, nonpreparative)  
 (in synthesis of azobenzene-linked diperphyrin Zn complexes)  
 RN 220213-37-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 69 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1998-805861 CAPLUS  
 DOCUMENT NUMBER: 130:189901  
 TITLE: Structure-optical property relationships of porphyrins  
 AUTHOR(S): Su, Weijie; Cooper, Thomas M.; Nguyen, Kiet; Brant, Mark C.; Brandelik, Donna; McLean, Daniel G.; Wright Laboratory, WL/MLPJ, Wright-Patterson AFB, OH, 45433, USA  
 CORPORATE SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1998), 3472(Nonlinear Optical Liquids for Power Limiting and Imaging), 136-143  
 SOURCE: CODEN: PSISDG; ISSN: 0277-786X  
 PUBLISHER: SPIE-The International Society for Optical Engineering  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Porphyrins are attractive compds. for optical applications. The authors were studying the relation between mol. structure and optical properties of a number of porphyrin compds. Structural variations explored include insertion of metal ions, extension of conjugation, halogenation and alkylation either at the pyrrole position or the meso-aryl groups. The characterization of these chromophores includes measurement of UV/visible, fluorescence and fluorescence lifetimes. Also, the authors have studied their nonlinear absorption, excitation dynamics. The significant factors influencing limiting behavior appear to be the heavy atom effect, electron donating and withdrawing substituents, conformation distortion and changes in conjugation. Detailed understanding will be gained from measurements of photophys. parameters underlying limiting behavior.  
 IT 120644-25-9 131214-86-3  
 RL: PRP (Properties)  
 (structure-optical property relationships of porphyrins)  
 RN 120644-25-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 69 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

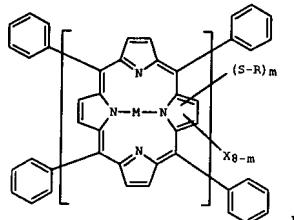


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

C1 Cl Rh C1  
 Cl C1 Ph C1  
 C1 C1 Ph C1  
 C1 C1 Ph C1  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

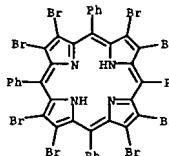
L6 ANSWER 70 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1998-795635 CAPLUS  
 DOCUMENT NUMBER: 130:102947  
 TITLE: Porphyrin compound and laser-recordable optical recording medium using it  
 INVENTOR(S): Masaoka, Toshihiro; Terao, Hiroshi; Kumagaya, Youjiro; Tsukahara, Hiroshi; Misawa, Tsutayoshi; Takuma, Keisuke  
 PATENT ASSIGNEE(S): Mitsui Chemicals Inc., Japan; Yamamoto Chemicals Inc.  
 SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.  
 CODEN: JKOKAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10330632	A2	19981215	JP 1997-138509	19970528
PRIORITY APPLN. INFO.:			JP 1997-138509	19970528
OTHER SOURCE(S):	MARPAT	130:102947		
GI				



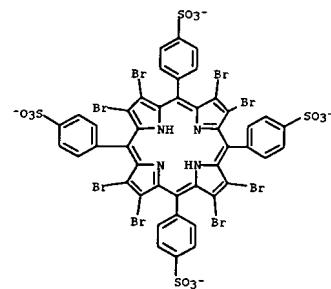
AB The porphyrin compound comprises I (R = alkyl, (un)substituted Ph, naphthyl, X = H, halo; m = 1-8; M = 2H, divalent metal, trivalent or tetravalent metal derivative). The recording medium has a recording layer containing I. The medium showed high sensitivity for 520-690-nm laser light.  
 IT 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (thioetherified porphyrin compound for laser-recordable optical recording medium)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 70 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L6 ANSWER 71 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1998-593206 CAPLUS  
 DOCUMENT NUMBER: 129:266109  
 TITLE: Kinetics and mechanism of the reaction of mercury(II) with a water-soluble octabromoporphyrin  
 AUTHOR(S): Nahar, N.; Tabata, M.  
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840, Japan  
 SOURCE: Journal of Porphyrins and Phthalocyanines (1998), 2(4-5), 397-403  
 CODEN: JPPHZ  
 ISSN: 1088-4246  
 PUBLISHER: John Wiley & Sons Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The reaction of mercury(II) hydroxide with 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin, (TPPSBr8)H24- (HgP4-), to form the mercury(II) porphyrin [(TPPSBr8)Hg]4- (HgP4-) was investigated in the pH range 6.2-8.5. The observed rate constant was first-order with respect to the mercury(II) concentration and decreased with increasing pH from pH 6.2 to 7.5 and then increased from pH 7.5 to 8.5. The rate expression was written as  $d[HgP4-]/dt = (KHPK-1[H+]-1 + KH2P + KH3PK[H+]) (1 + K1[H+] + K-1[H+]-1 - [Hg(OH)2][H2P4-])$ . The KHP, KH2P and KH3PK values were found to be  $(1.33 \pm 0.02) \times 10^6$ ,  $(5.50 \pm 0.08) \times 10^6$  and  $(1.40 \pm 0.08) \times 10^8$  M<sup>-1</sup> s<sup>-1</sup> resp., with  $K1 = [HgP3-][H2P4-]-1[H+]-1 = 104.83 \pm 0.04$  and  $K-1 = [HgS-][H+][H2P4-]-1 = 1010.02 \pm 0.02$ . The activation parameters were  $\Delta H_{\text{P,thermod.}} = 94 \pm 12$  kJ mol<sup>-1</sup> and  $\Delta S_{\text{P,thermod.}} = 226 \pm 22$  J K<sup>-1</sup> mol<sup>-1</sup> for the KHP path,  $\Delta H_{\text{H3PK,thermod.}} = 31 \pm 4$  kJ mol<sup>-1</sup> and  $\Delta S_{\text{H3PK,thermod.}} = -6.4 \pm 0.4$  J K<sup>-1</sup> mol<sup>-1</sup> for the KH2P path and  $\Delta H_{\text{H2PK,thermod.}} = 40 \pm 7$  kJ mol<sup>-1</sup> and  $\Delta S_{\text{H2PK,thermod.}} = 44 \pm 4$  J K<sup>-1</sup> mol<sup>-1</sup> for the KH3PK path. The kinetic results show the high reactivity of mercury(II) hydroxide towards the protonated porphyrin.  
 IT 176173-80-1 CAPLUS  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
 (kinetics and mechanism of reaction of mercury(II) with water-soluble octabromoporphyrin)  
 RN 176173-80-1 CAPLUS  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis-, ion(4-) (9CI) (CA INDEX NAME)

L6 ANSWER 71 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

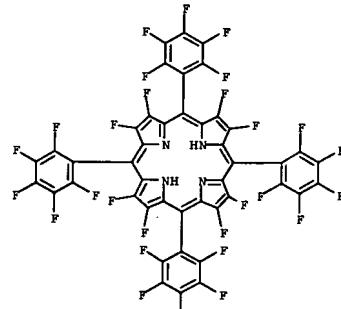
L6 ANSWER 72 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1998-577480 CAPLUS  
 DOCUMENT NUMBER: 129-253965  
 TITLE: *19F NMR and Structural Evidence for Spin-State Modulation of Six-Coordinate Cobalt(II) in a Weak Field Porphyrin Ligand*  
 AUTHOR(S): Smirnov, Valeriy V.; Woller, Eric K.; DiMaggio, Stephen G.  
 CORPORATE SOURCE: Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE, 68588-0304, USA  
 SOURCE: Inorganic Chemistry (1998), 37(19), 4971-4978  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The syntheses and characterization of [2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenylporphyrinato]cobalt, Co(F28TPP), and [2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrinato]cobalt, Co(F28TPP)-2Ph, are reported. Co(F28TPP)-2Ph (tol = toluene) crystallizes in the monoclinic space group C<sub>h</sub> with a 22.1616(5), b 12.0274(3), c 19.9159(2) Å,  $\beta$  110.645(1) $^\circ$ , and  $Z$  = 4 (dcalcd = 1.818 g/cm<sup>3</sup>;  $\mu$ (Mo K $\alpha$ ) = 0.50 mm<sup>-1</sup>), and Co(F28TPP)-2THF crystallizes in the triclinic space group P-1 with a 11.0691(1), b 12.0451(1), c 12.9558(2) Å,  $\alpha$  62.531(1),  $\beta$  69.544(1),  $\gamma$  76.181(1) $^\circ$ , and  $Z$  = 1 (dcalcd = 1.700 g/cm<sup>3</sup>;  $\mu$ (Mo K $\alpha$ ) = 0.45 mm<sup>-1</sup>). A comparison of the x-ray crystal structure data from Co(F28TPP)-2tol and Co(F28TPP)-2THF indicates that the porphyrin core expands dramatically (0.08 Å) in the six-coordinate complex. Optical and <sup>19</sup>F NMR spectroscopic studies of Co(F28TPP) in the presence of added ligand demonstrate that spin-state modulation of the six-coordinate Co(II) center is facile. Partial population of the 4Eg state is accessed upon coordination of the cobalt center with THF  $\sigma$ -donor ligands, while six-coordinate complexes with 1-methylimidazole result in complete conversion to the high spin state, as evinced by 280 ppm downfield chemical shifts for the  $\beta$ -fluorine resonances in the <sup>19</sup>F NMR spectrum. Co(F28TPP) is the 1st example of a porphyrin which supports a high-spin cobalt ion.

IT 121399-88-0, 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphine 186885-28-9, 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetraphenylporphine  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (for preparation of cobalt fluorinated tetraphenylporphyrinato complexes)  
 RN 121399-88-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

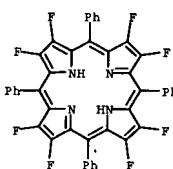
L6 ANSWER 72 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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RN 186885-28-9 CAPLUS  
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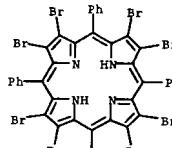
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 73 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1998-577449 CAPLUS  
 DOCUMENT NUMBER: 129-269434  
 TITLE: *Electronic, Spectral, and Electrochemical Properties of (TPPB<sub>x</sub>)Zn Where TPPB<sub>x</sub> Is the Dianion of  $\beta$ -Brominated-Pyrrole Tetraphenylporphyrin and x Varies from 0 to 8*  
 AUTHOR(S): D'Souza, Francis; Zandler, Melvin E.; Tagliatesta, Pietro; Ou, Zhongping; Shao, Jianguo; Van Caemelbeke, Eric; Kadish, Karl M.  
 CORPORATE SOURCE: Department of Chemistry, Wichita State University, Wichita, KS, 67260-0051, USA  
 SOURCE: Inorganic Chemistry (1998), 37(18), 4567-4572  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The electronic, spectral, and electrochem. characterization of (meso-tetraphenylporphyrinato)zinc(II) complexes bearing between 0 and 8 bromo substituents at the  $\beta$ -pyrrole positions is reported. The studied compds. are represented as (TPPB<sub>x</sub>)Zn where TPPB<sub>x</sub> is the dianion of brominated 5,10,15,20-tetraphenylporphyrin and x varies between 0 and 8. Each porphyrin undergoes four well-defined 1-electron transfer reactions to yield porphyrin  $\pi$ -cation radicals and dianions upon oxidation and porphyrin  $\pi$ -anion radicals and dianions upon reduction. Half-wave potentials for the 1st reduction of (TPPB<sub>x</sub>)Zn can be described by a single linear free energy relation, and plots of E<sub>1/2</sub> vs. the number of Br groups on the complex show a linear correlation with a pos. slope of 63 mV per Br group. This is not the case for the other three electron transfer processes of the compds. where plots of E<sub>1/2</sub> vs. the number of Br groups show distinctly different linear correlations for derivs. with 0-4 Br groups and those with 4-8 Br groups. The effect of increasing number of Br groups on the spectral and electrochem. properties of the neutral complexes was examined over the whole series of compds., and these exptl. results are compared to results of theor. calcns. by semiempirical MO AM1 methods using configurational interactions (CI) over the four Gouterman frontier  $\pi$ -orbitals. The dihedral angle containing the four porphyrin macrocycle ring nitrogens is proposed as a measure of porphyrin ring nonplanarity, and this value increases with increasing number of Br substituents on (TPPB<sub>x</sub>)Zn. Results of the AM1-CI calcns. indicate that the spectrally determined HOMO-LUMO gap, i.e., the energy corresponding to the low-energy absorption band, varies in a nonlinear fashion with increasing number of Br substituents on the macrocycle and this is due to both the electronic effect of the substituents and the macrocycle nonplanarity. The HOMO-LUMO gaps theor. calculated by AM1-CI = 4 methods thus parallel values which are exptl. obtained by electrochem. or spectroscopy. The lack of well-defined linear free energy relations for all processes except for the 1st reduction can be explained from electronic effects caused by the halogen substituents and nonplanar macrocyclic distortions induced by steric interactions among the peripheral substituents. In the case of porphyrin dication formation, the redox potentials are virtually independent of the bromo substituents.

IT 131214-86-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (for preparation of zinc brominated tetraphenylporphyrinato complex)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 73 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

DOCUMENT NUMBER: 129:269428

TITLE: Novel covalently linked porphyrin trimers with redox-distinct properties  
AUTHOR(S): Sen, Avijit; Anandhi, U.; Krishnan, V.

CORPORATE SOURCE: Chemical Biology unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560 012, India

SOURCE: Tetrahedron Letters (1998), 39(36), 6539-6542

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

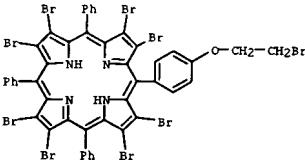
AB Two novel porphyrin trimers bearing different metal centers and/or different peripheral substituents were synthesized. These systems display interesting spectral and electrochem. redox properties.

IT 213414-00-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(for preparation of ethanedioxy-linked tetraphenylporphyrin trimer)

RN 213414-00-7 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-[4-(2-bromoethoxy)phenyl]-10,15,20-triphenyl- (9CI) (CA INDEX NAME)



IT 213482-55-4P

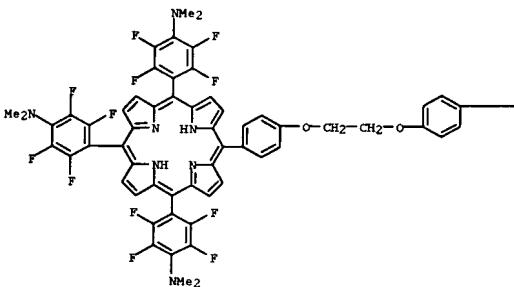
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation, cyclic voltammetry, NMR and electronic absorption spectra,

and fluorescence quenching)

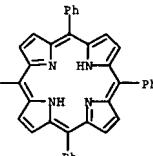
RN 213482-55-4 CAPLUS

CN Benzenamine, 4,4',4''-[20-[4-[2-[4-[C-[3,5-dimethyl-4-[2-[4-(2,3,7,8,12,13,17,18-octabromo-10,15,20-triphenyl-21H,23H-porphin-5-yl)phenoxy]ethoxy]phenyl]-10,15,20-triphenyl-21H,23H-porphin-5-yl]phenoxy]ethoxy]phenyl]-21H,23H-porphine-5,10,15-triyl]tris[2,3,5,6-tetrafluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

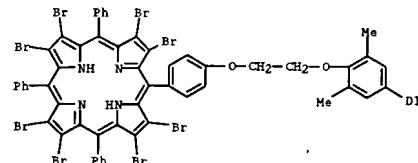
PAGE 1-A



PAGE 1-B



PAGE 2-A



DOCUMENT NUMBER: 129:260548

TITLE: Novel 1,2-Rearrangement of Porphyrinatorhodium(III) Alkyls: Cis  $\beta$ -Hydride Elimination/Olefin

Metal-Hydride Insertion Pathway

AUTHOR(S): Mak, Kin Wah; Chan, Kin Shing  
COPORATE SOURCE: Department of Chemistry, The Chinese University of Hong Kong, Shatin, Hong Kong

SOURCE: Journal of the American Chemical Society (1998), 120 (37), 9686-9687

CODEN: JACSAU; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB  $Rh(boc)_3R$  ( $boc = 5,10,15,20$ -tetrakis-(4'-tert-butylphenyl)-2,3,7,8,12,13,17,18-octachloroporphyrinate;  $R = CH_2CH_2C_6H_4X-p$ ;  $X = NO_2$ , Cl, H, Me, OMe) were prepared and their thermal isomerization to  $Rh(boc)_3R'$  ( $R' = CH_2CH_2C_6H_4X-p$ ) was studied. The authors deduced a cis  $\beta$ -hydride elimination/olefin metal-hydride insertion pathway. The equilibrium constant and

kinetics parameters, including deuterium kinetic isotope effect, were determined

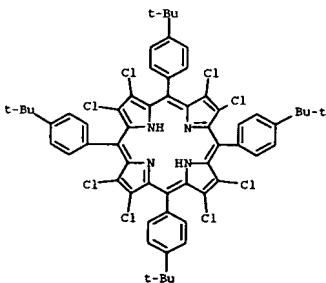
IT 213481-24-4P, 5,10,15,20-Tetrakis-(4-tert-butylphenyl)-

2,3,7,8,12,13,17,18-octachloroporphyrin

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate for preparation of rhodium tetraaryloctachloroporphyrinato phenylethyl complexes)

RN 213481-24-4 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1998:465549 CAPLUS

DOCUMENT NUMBER: 129:130641

TITLE: Spectrophotometric determination of lithium ion using a water-soluble octabromoporphyrin in aqueous solution

AUTHOR(S): Tabata, M.; Nishimoto, J.; Kusano, T.

CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840, Japan

SOURCE: Talanta (1998), 46(4), 703-709

CODEN: TLNTA2; ISSN: 0039-9140

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A water-soluble porphyrin, (2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonophenyl)porphyrin, H<sub>2</sub>obtpps<sub>4</sub><sup>-</sup>) was synthesized and developed for the determination of Li<sup>+</sup> ion in aqueous solution. The octabromo groups lower the basicity of the porphyrin by their electron-withdrawing effect, and enable the porphyrin to react with the Li<sup>+</sup> ion in alkaline solution to form the Li<sup>+</sup>

complex along with a shift of absorption maximum: A maximum/nm (log ε/mol<sup>-1</sup> dm<sup>3</sup> cm<sup>-1</sup>) of the Li<sup>+</sup> porphyrin are 490.5 nm (5.31) and 734 nm (4.36). Na<sup>+</sup> and K<sup>+</sup> ions did not react with the porphyrin. The equilibrium constant for the reaction Li<sup>+</sup> + H<sub>2</sub>obtpps<sub>4</sub><sup>-</sup> ⇌ [Li(H<sub>2</sub>obtpps<sub>4</sub><sup>-</sup>)]<sup>5-</sup> + H<sup>+</sup> is 10<sup>-8.80</sup> and the conditional formation constant of the [Li(H<sub>2</sub>obtpps<sub>4</sub><sup>-</sup>)]<sup>5-</sup> at pH 13 is 104.21. The above results were applied to the determination of Li<sup>+</sup>

ion in aqueous solution. The interference from transition and heavy metal ions was masked by using N,N'-1,2-ethanediybis[N(carboxymethyl)glycinate]magnesium (II) ([Mg(EDTA)]<sub>2</sub><sup>-</sup>) solution. Absorbance at 490 nm was measured against a blank solution. A calibration graph was linear at 0.007-0.7 μg cm<sup>-3</sup> (1 + 10<sup>-6.1</sup> + 10<sup>-4</sup> mol dm<sup>-3</sup>) of Li<sup>+</sup> (I) with a correlation factor of 0.967. Li<sup>+</sup> ion less than ppm level was determined spectrophotometrically

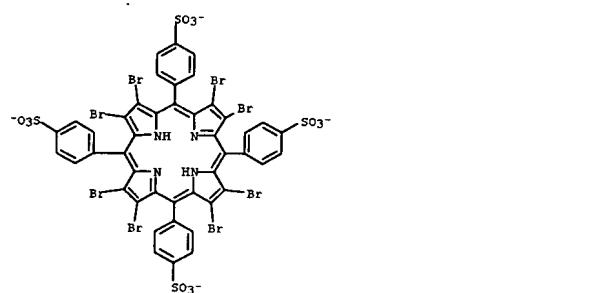
in aqueous solution. The proposed method was applied to the determination of Li<sup>+</sup> in human serum and sea water samples.

IT 176173-80-1P. 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetrakis(4-sulfonophenyl)porphyrin

RL: ARI (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses) (spectrophotometric determination of lithium ion using a water-soluble octabromoporphyrin in aqueous solution)

RN 176173-80-1 CAPLUS

CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis-, ion(4-) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1998:401896 CAPLUS

DOCUMENT NUMBER: 129:154264

TITLE: Fast atom bombardment mass spectral observations on some β-halogenated tetraphenylporphyrins and their iron derivatives. [Erratum to document cited in CA128:250176]

AUTHOR(S): Boschi, Tristano; D'Arcangelo, Giuseppe; Tagliatesta, Pietro

CORPORATE SOURCE: Dip. Scienze Tecnologiche Chimiche, Universita Studi Roma "Tor Vergata", Rome, 00173, Italy

SOURCE: European Mass Spectrometry (1998), 4(1), 83

CODEN: EMSPFW; ISSN: 1356-1049

PUBLISHER: IM Publications

DOCUMENT TYPE: Journal

LANGUAGE: English

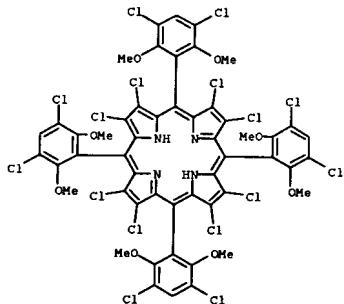
AB The captions for Figures 5, 6, and 7 and for Figures 8 and 9 were transposed in press; the correct captions are given.

IT 180711-85-7

RL: PRP (Properties) (fast atom bombardment mass spectral observations on β-halogenated tetraphenylporphyrins and iron derivs. (Erratum))

RN 180711-85-7 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1998:381712 CAPLUS

DOCUMENT NUMBER: 128:322841

TITLE: Peroxide Decoloration of Azo Dyes Catalyzed by Polyethylene Glycol-Linked Manganese Halogenated Porphyrins

AUTHOR(S): Nango, Mamoru; Iwasaki, Toyota; Takeuchi, Yoshito; Kurono, Yukihisa; Tokuda, Junko; Oura, Ritsuko

CORPORATE SOURCE: Department of Applied Chemistry, Nagoya Institute of Technology, Nagoya, 466, Japan

SOURCE: Langmuir (1998), 14(12), 3272-3278

CODEN: LANGD5; ISSN: 0743-7463

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Polyethylene glycol (PEG)-linked manganese halogenated porphyrins (Chart 1) catalyzed oxidation of azo dyes (Chart 2) by H<sub>2</sub>O<sub>2</sub> under mild conditions such as pH 8.0 at 25 °C especially when imidazole was present, causing the decoloration of azo dyes. The decoloration of azo dyes by synthetic manganese porphyrins under mild conditions was first reported. The decoloration rate depended on the structures of the porphyrins, in which the largest rate was observed in the presence of PEG-MnCPP. The decoloration may be contributed by radical species rather than electrophilic species, consistent with the side-chain oxidation of toluene. Kinetics on polyethylene glycol-linked manganese porphyrin-catalyzed decoloration of C.I. Acid Orange 7 by hydrogen peroxide revealed that the decoloration was contributed at the oxidation process by manganese porphyrins

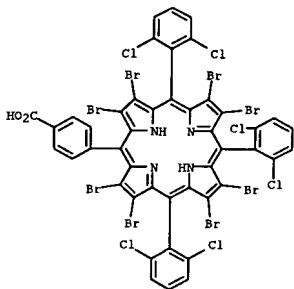
with hydrogen peroxide in the polymer domain rather than the complex-formation process between manganese porphyrins and azo dyes.

IT 206987-42-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate for catalysts; peroxide decoloration of azo dyes catalyzed by polyethylene glycol-linked manganese halogenated porphyrins)

RN 206987-42-0 CAPLUS

CN Benzoic acid, 4-[2,3,7,8,12,13,17,18-octabromo-10,15,20-tris(2,6-dichlorophenyl)-21H,23H-porphin-5-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1998-336754 CAPLUS

DOCUMENT NUMBER: 129-67628

TITLE: Ab initio calculations on porphyrins in the condensed phase

AUTHOR(S): Day, P. N.; Wang, Z.; Pachter, R.

CORPORATE SOURCE: Materials Directorate, Air Force Research Laboratory, Wright-Patterson AFB, OH 45433, USA

SOURCE: Materials Research Society Symposium Proceedings (1998), 488 (Electrical, Optical, and Magnetic Properties of Organic Solid-State Materials IV), 853-858

CODEN: MRSPPH; ISSN: 0272-9172

PUBLISHER: Materials Research Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Porphyrins are a promising class of materials for optical limiting applications, and in the condensed phase solvent effects have been shown to be significant. The authors report results with a method designed to simulate the effects of discrete solvent mol., namely the effective fragment potential (EFP) approach which has been implemented for use in ab initio calcs. Further, a simulated annealing (SA) method has been implemented with the EFP solvation model in an attempt to solve the problem of multiple min. in clusters of molis. The results with this method indicate some success on models of aqueous formamide and aqueous glutathione.

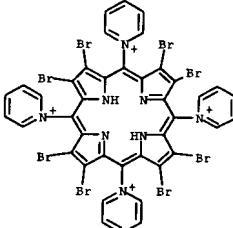
acid. Ab initio calcs. can now be carried out on porphyrins, and the solvation methods are being updated for their use on these systems.

IT 208995-40-8

RL: PRP (Properties)  
(ab initio calcs. on octabromotetraphyrin porphyrin cation in the condensed phase)

RN 208995-40-8 CAPLUS

CN Pyridinium, 1,1',1'',1'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis- (9Cl) (CA INDEX NAME)



REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1998-302287 CAPLUS

DOCUMENT NUMBER: 129-59211

TITLE: Saddle-shaped dioxo-ruthenium(VI) and -osmium(VI) 2,3,5,7,8,10,12,13,15,17,18,20-dodecaphenylporphyrin (H2dpp) complexes. Synthesis, spectral characterization and alkene oxidation by [RuVI(dpp)O2]

AUTHOR(S): Liu, Chun-Jing; Yu, Wing-Yiu; Peng, Shie-Ming; Mak, Thomas C. W.; Che, Chi-Ming

CORPORATE SOURCE: Department of Chemistry, The University of Hong Kong, Hong Kong

SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1998), (11), 1805-1812

CODEN: JCDTB1; ISSN: 0300-9246

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An improved procedure for the preparation of the saddle-distorted porphyrin 2,3,5,7,8,10,12,13,15,17,18,20-dodecaphenylporphyrin (H2dpp) (yield = 75%) based on the Suzuki cross-coupling reaction between phenylboronic acid PhB(OH)2 and [2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin] has been developed. X-Ray diffraction studies of [MII(dpp)(CO)(py)] (M = Ru 1 or Os 3) showed that 1 and 3 are isostructural, and the porphyrin macrocycles exhibit severe out-of-plane saddle and ruffle distortions. In both 1 and 3 the pyrrole rings are alternately tilted up and down with respect to the least-squares plane of the 25-atom porphyrin core, and the pyrrole carbons experience an average displacement of 0.769 Å from the least-squares plane compared to 0.78 Å for free H2dpp, whereas the Ru and Os atoms are displaced by 0.1006 and 0.0792 Å from the 25-atom porphyrin core resp. The complex [RuVI(dpp)O2] 2, prepared by m-chloroperoxybenzoic acid oxidation, is an active

oxidant for alkene epoxidns. in CH2Cl2 [containing 2% (weight/weight) pyrazole].

styrene, norbornene and cis-stilbene were oxidized selectively to their resp. epoxides in excellent yield. Complete stereoretention was observed

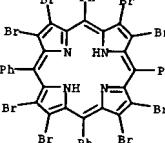
for the oxidation of cis-stilbene, however oxidation of cis- $\beta$ -methylstyrene afforded significant amts. of trans-epoxide suggesting that a carboradical mechanism is operative. The crystal structure of the complex [RuVI(dpp)2] 5, the product of the stoichiometric alkene oxidns., was determined. Magnetic susceptibility measurement ( $\mu_{eff}$  = 3.24  $\mu_B$ ) suggests the formulation of RuIV with two unpaired electrons in its electronic ground state. The Ru-N (pz) bond distances are 2.022(13) and 2.083(12) Å. The reactions of 2 with alkenes in CH2Cl2 (with 2% Hzp) follow second-order kinetics: rate =  $k_1[2][alkene]$ . For norbornene and styrene, the second-order rate consts.,  $k_1$ , in CH2Cl2 at 25.9 °C are  $(3.79 \pm 0.04) \times 10^{-3}$  and  $(4.78 \pm 0.09) \times 10^{-3}$  dm<sup>3</sup> mol<sup>-1</sup> s<sup>-1</sup> resp.

IT 131214-86-3 [2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin]

RL: RCT (Reactant); RACT (Reactant or reagent) (saddle-shaped dioxo-ruthenium(VI) and -osmium(VI) 2,3,5,7,8,10,12,13,15,17,18,20-dodecaphenylporphyrin (H2dpp) complexes and synthesis, spectral characterization and alkene oxidation by [RuVI(dpp)O2])

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9Cl) (CA INDEX NAME)



REFERENCE COUNT:

40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 81 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1998:269879 CAPLUS  
DOCUMENT NUMBER: 128:328423

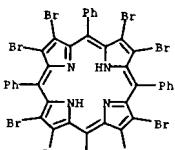
TITLE: Investigation of Reverse-Saturable Absorption in  
Brominated Porphyrins  
AUTHOR(S): Su, Weijie; Cooper, Thomas M.; Brant, Mark C.  
CORPORATE SOURCE: Air Force Research Laboratory AFRL/MLPJ,  
Wright-Patterson Air Force Base, Dayton, OH, 45433,  
USA  
SOURCE: Chemistry of Materials (1998), 10(5), 1212-1213  
CODEN: CMATEK; ISSN: 0897-4756  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Nonlinear absorption data are given for both octabromotetraphenylporphyrin (H2OBP) and some metallocabromotetraphenylporphyrins (MOBP). ZnOBP had strong nonlinear absorption comparable to state-of-the-art phthalocyanine dyes.

IT 131214-86-3

RL: PRP (Properties)  
(reverse-saturable absorption in)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-  
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 82 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1998:250205 CAPLUS  
DOCUMENT NUMBER: 128:316734

TITLE: Application of matrix-assisted laser desorption/ionization Fourier transform mass spectrometry to the analysis of planar porphyrins and highly substituted nonplanar porphyrins  
AUTHOR(S): Green, M. Kirk; Medforth, Craig J.; Muzzi, Cinzia M.; Nurco, Daniel J.; Shea, Kalyan M.; Smith, Kevin M.; Lebrilla, Carlito B.; Shelutt, John A.

CORPORATE SOURCE: Department of Chemistry, University of California at Davis, Davis, CA, 95616, USA  
SOURCE: European Mass Spectrometry (1997), 3(6), 439-451  
CODEN: EMSPFW; ISSN: 1356-1049

PUBLISHER: IM Publications  
DOCUMENT TYPE: Journal  
LANGUAGE: English

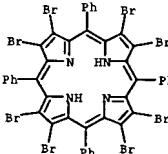
AB The applicability of matrix-assisted laser desorption/ionization (MALDI) Fourier transform mass spectrometry to the anal. of porphyrins was examined. High resolution spectra were readily obtained with good sensitivity and a detection limit  $\approx$  2 fmol. A mixed solvent system of toluene and ethanol (1: 1 by volume) proved to be compatible with the 2,5-dihydroxybenzoic acid (DHB) matrix and solubilized most of the porphyrins examined. Porphyrins which were insol. in this solvent mixture could be dissolved in an appropriate solvent and deposited on a layer of DHB (layered MALDI). The parent ion was generally the largest peak in the spectrum, although for some metallocporphyrins the peak corresponding to (M - metal + 3H)<sup>+</sup> was dominant. The extent of demetalation depends on factors such as sample preparation, the metal ion and the laser intensity. Addition of more than one hydrogen occurred in many cases but was a minor process. Spectra of compds. ionized by different methods showed increasing fragmentation in the order MALDI < layered MALDI < fast-atom bombardment < laser desorption.

IT 131214-86-3 206349-60-2

RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)  
(MALDI Fourier transform mass spectrometry in anal. of planar porphyrins and highly substituted nonplanar porphyrins and their metal complexes)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-  
(9CI) (CA INDEX NAME)

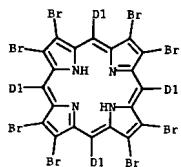
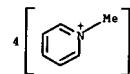


RN 206349-60-2 CAPLUS

CN Pyridinium, (2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[1-methyl-, tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

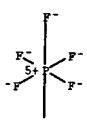
L6 ANSWER 82 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
CM 1

CRN 206349-59-9  
CMF C44 H30 Br8 N8  
CCI IDS



CM 2

CRN 16919-18-9  
CMF F6 P  
CCI CCS



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 83 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1998:131988 CAPLUS  
DOCUMENT NUMBER: 128:250176

TITLE: Fast atom bombardment mass spectral observations on some  $\beta$ -halogenated tetraphenylphosphorins and their iron derivatives  
AUTHOR(S): Boschi, Tristano; D'Arcangelo, Giuseppe; Tagliatesta, Pietro

CORPORATE SOURCE: Dip. Scienze Tecnologie Chimiche, Universita Studi Roma "Tor Vergata", Rome, I-00173, Italy  
SOURCE: European Mass Spectrometry (1997), 3(5), 355-360  
CODEN: EMSPFW; ISSN: 1356-1049

PUBLISHER: IM Publications  
DOCUMENT TYPE: Journal  
LANGUAGE: English

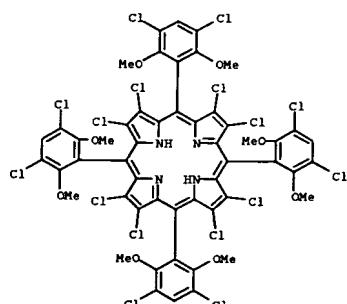
AB The fast atom bombardment mass spectral observations on some  $\beta$ -halogenated tetraphenylporphyrins and their iron derivs. were compared in order to investigate the relative stability of these complexes. The investigated compds. are represented as O[FeBr4TPP]<sub>2</sub>, O[FeTPP(4-Br)]<sub>2</sub>, O[FeTPP(4-OCH<sub>3</sub>)]<sub>2</sub>, H<sub>2</sub>[Br4TPP], Fe[Br4TPP]Cl, H<sub>2</sub>(Cl16TDCMPP) and Fe(Cl16TDCMPP)Cl where Br4TPP is the dianion of 7,8,17,18-tetrabromo-5,10,15,20-tetraphenylphosphyrin, TPP(4-Br) is the dianion of 5,10,15,20-tetraphenylporphyrin, TPP(4-Br) is the dianion of 5,10,15,20-tetra(4-bromo)phenylporphyrin, TPP(4-OCH<sub>3</sub>) is the dianion of 5,10,15,20-tetra(4-methoxy)phenylporphyrin and Cl16TDCMPP is the dianion of 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetra(2,6-dimethoxy-3,5-dichlorophenyl)porphyrin. The stability of each mol. ion and the subsequent fragmentations were correlated to the substitution of the porphyrin rings and to the loss of steric hindrance.

IT 180711-85-7

RL: PRP (Properties)  
(fast atom bombardment mass spectral observations on  $\beta$ -halogenated tetraphenylphosphorins and iron derivs.)

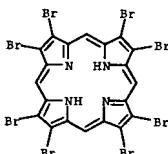
RN 180711-85-7 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 83 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

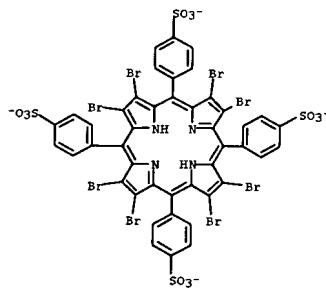
L6 ANSWER 84 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1998:99309 CAPLUS  
 DOCUMENT NUMBER: 128:132114  
 TITLE: Lithium(I) porphyrin complex for the spectrophotometric determination of lithium ion in aqueous solution  
 AUTHOR(S): Tabata, Masaaki; Kusano, Tohru; Nishimoto, Jun  
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840, Japan  
 SOURCE: Analytical Sciences (1997), 13(Suppl., Asiananalysis IV), 157-160  
 PUBLISHER: CODEN: ANSCEN; ISSN: 0910-6340  
 DOCUMENT TYPE: Japan Society for Analytical Chemistry  
 LANGUAGE: Journal  
 English  
 AB A water-soluble octabromoporphyrin was synthesized for the determination of Li in water. The porphyrin reacts with Li in alkaline solution to form the Li complex along with a shift of absorption maximum to shorter wave length. Na and K ions do not react with the porphyrin. The equilibrium constant of the Li(I) porphyrin complex was determined and applied to the determination of Li in natural water. Interference of metal ions was removed by ligand buffer of Mg-EDTA complex.  
 IT 144811-83-6  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (lithium porphyrin complex for spectrophotometric determination of lithium in water)  
 RN 144811-83-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



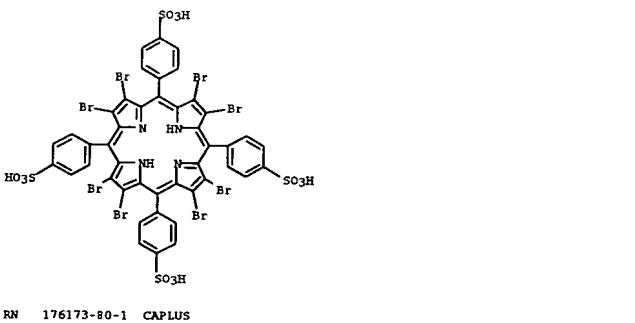
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 85 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1998:99297 CAPLUS  
 DOCUMENT NUMBER: 128:249140  
 TITLE: Ion-pair extraction of lithium ion by a water-soluble porphyrin  
 AUTHOR(S): Haiping, Sun; Nishimoto, Jun; Tabata, Masaaki  
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840, Japan  
 SOURCE: Analytical Sciences (1997), 13(Suppl., Asiananalysis IV), 119-122  
 PUBLISHER: CODEN: ANSCEN; ISSN: 0910-6340  
 DOCUMENT TYPE: Japan Society for Analytical Chemistry  
 LANGUAGE: Journal  
 AB The equilibrium of ion-pair extraction of lithium porphyrin [octabromoporphyrin: 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin, H2obtpp94- H24-] with tetrabutylammonium (X+) was studied at 25° and I = 0.1 (NaCl, NaOH). Extraction and dissociation constants of the ion-pair complexes of free base porphyrin, deprotonated porphyrin and lithium porphyrin, defined as  $K_{ex}(H2P) = [H2P]^{+}a[X+]^{4+}$ ,  $K_{ex}(HP) = [X5HP]^{+}a/[HP5]^{+}a[X+]^{4+}$ ,  $K_{ex}(LiP) = [LiP]^{+}a[X+]^{4+}$ ,  $K_{dis}(H2P) = [H3H2P-]^{+}a[X+]^{4+}/[H2P]^{+}a[X+]^{4+}$ ,  $K_{dis}(LiP) = [LiP]^{+}a[X+]^{4+}/[LiP]^{+}a[X+]^{4+}$ ,  $K_{dis}(HP) = [X5HP]^{+}a[X+]^{4+}/[X4HP]^{+}a[X+]^{4+}$  and  $K_{dis}(LiP) = [X5LiP]^{+}a[X+]^{4+}/[X4LiP]^{+}a[X+]^{4+}$ , were determined. These values were found to be  $K_{ex}(H2P) = (9.5 \pm 1.5) + 1013$  (mol-4dm<sup>-3</sup>),  $K_{dis}(H2P) = (3.5 \pm 0.7) + 10^{-1}$  (mol dm<sup>-3</sup>),  $K_{ex}(HP) = (4.7 \pm 0.4) + 1016$  (mol-5dm<sup>-3</sup>), and  $K_{ex}(LiP) = (1.4 \pm 0.7) + 1012$  (mol-4dm<sup>-3</sup>), resp.  
 IT 154783-99-0, lithium tetrabutylammonium salts 176173-80-1  
 RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)  
 (ion-pair extraction of lithium ion by water-soluble porphyrin)  
 RN 154783-99-0 CAPLUS  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetraysl)tetraakis- (9CI) (CA INDEX NAME)

L6 ANSWER 85 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetraysl)tetraakis-, ion(4-) (9CI) (CA INDEX NAME)

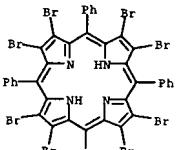


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



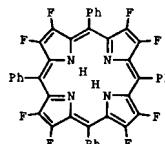
RN 176173-80-1 CAPLUS

L6 ANSWER 86 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1998:33809 CAPLUS  
 DOCUMENT NUMBER: 128:167041  
 TITLE: DFT study of alkynylporphyrin dimers and brominated tetraphenylporphyrins  
 AUTHOR(S): Wang, Zhiqiang; Day, Paul; Pachter, Ruth; McLean, Daniel G.  
 CORPORATE SOURCE: Materials Directorate, Wright Laboratory, WL/MLP  
 Wright-Patterson Air Force Base, OH, 45433-7702, USA  
 SOURCE: Materials Research Society Symposium Proceedings (1997), 479 (Materials for Optical Limiting II), 331-336  
 CODEN: MRSDDH; ISSN: 0272-9172  
 PUBLISHER: Materials Research Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Geometry optimizations and electronic structure calcns. using D. Functional Theory (DFT) are reported for tetracyclyleneporphyrins (TAP), their dimers, and octabromotetraphenylporphyrins (OBP). The acetylene group contributes to the  $\beta$ -electron conjugation along the porphyrin ring for the HOMO and LUMO, and reduces significantly the HOMO-LUMO gap. The gap is further reduced in dimers. The planar geometry of the TAP dimer has a lower energy than the non-planar one. The geometry of H2OBP is found to be non-planar, and the distortion of porphyrin ring is shown to be closely related to the HOMO-LUMO gap.  
 IT 131214-86-3  
 RL: PRP (Properties); (DFT study of alkynylporphyrin dimers and brominated tetraphenylporphyrins)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

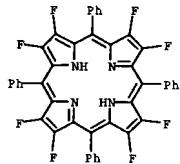
L6 ANSWER 87 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1997:780194 CAPLUS  
 DOCUMENT NUMBER: 128:75218  
 TITLE: 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenylporphyrin: first synthesis and x-ray crystal structure of the ZnII complex  
 AUTHOR(S): Laroche, Jacques; Bondon, Arnaud; Toupet, Loic; Roland, Christian  
 CORPORATE SOURCE: Ecole Normale Supérieure. Département de Chimie, URA CNRS 1679, Paris, F-75231, Fr.  
 SOURCE: Chemistry—A European Journal (1997), 3 (11), 1890-1893  
 CODEN: CEUEBD; ISSN: 0947-6539  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 G1



I

AB 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetraphenylporphyrin (I) was prepared from 3,4-difluoropyrrole and benzaldehyde under Lindsey conditions. An X-ray crystal structure study of its ZnII complex has shown that the macrocycle core is nonplanar, a result in apparent contradiction with a blue-shifted UV/Vis spectrum. The results reported here demonstrate that a wide range of  $\beta$ -octafluoro-meso-arylated porphyrins, a new class of highly electron-deficient ligands, are potentially accessible from 3,4-difluoropyrrole, thus opening the door to, inter alia, efficient and robust oxidation catalysts.  
 IT 186885-28-9P, 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetraphenylporphyrin  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); (Preparation of octafluorotetraphenylporphyrin and the x-ray crystal structure of its zinc complex)  
 RN 186885-28-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 87 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

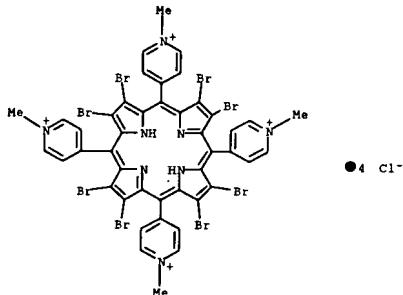
L6 ANSWER 88 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1997:723523 CAPLUS  
 DOCUMENT NUMBER: 128:7724  
 TITLE: Aggregation and axial ligand exchange behavior of water-soluble pyrrole- $\beta$  brominated porphyrins  
 AUTHOR(S): D'souza, Francis; Deviprasad, Gollapalli R.; Zandler, Melvin E.  
 CORPORATE SOURCE: Department of Chemistry, The Wichita State University, Wichita, KS, 67260-0051, USA  
 SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1997), (20), 3699-3703  
 CODEN: JCTBII; ISSN: 0300-9246  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Synthesis of two water-soluble pyrrole- $\beta$  brominated porphyrins, the tetrachloro salt of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(N-methyl-4-pyridinio)porphyrin [tetrakis(N-Me pyridyl)- $\beta$ -octabromo-porphyrin, (Br8TPyP)H2] and the tetrasodium salt of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis-(Ph sulfonato)porphyrin [tetrakis(4-sulfonatophenyl)- $\beta$ -octabromoporphyrin, (Br8TPPS)H2] and their zinc(II) derivs. are reported. The investigated porphyrins are highly nonplanar due to the presence of eight bromo substituents at the pyrrole- $\beta$  positions and four aryl groups at the meso positions. At  $T = -0.18$  and  $T = 23^\circ$ , the two sulfonated derivs., (Br8TPPS)H2 and (Br8TPPS)Zn show a small tendency to aggregate while such behavior is almost negligible for the N-Me pyridyl derivs. Like the unbrominated water-soluble zinc(II) porphyrin derivs., the pyrrole- $\beta$  brominated zinc(II) porphyrins, with one or two water mols. as axial ligand(s) in aqueous

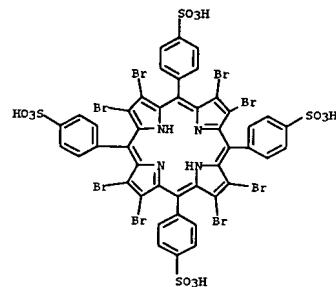
solution, undergo ligand exchange reactions with nitrogenous bases. The calculated equilibrium constant,  $K$ , for this reaction is smaller in magnitude when compared to that obtained for the corresponding unbrominated zinc(II) porphyrin derivs. The equilibrium constant values parallel the basicity of the axial ligands.

IT 186959-00-1P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); (preparation and absence of aggregation behavior in aqueous solution)  
 RN 186959-00-1 CAPLUS  
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[1-methyl-, tetrachloride, monohydrochloride (9CI) (CA INDEX NAME)

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● HCl

IT 198959-02-3P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and aggregation behavior in aqueous solution)  
 RN 198959-02-3 CAPLUS  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrasodium salt (9Cl) (CA INDEX NAME)

REFERENCE COUNT:

58

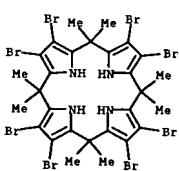
THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PAGE 2-A

●4 Na

L6 ANSWER 89 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 was described. Such macrocycles have proved to be effective and selective ion- and neutral mol.-binding agents forming supramol. ensembles, and ion- and neutral mol.-sepn. agents. The macrocycles are fully meso-non-hydrogen-substituted porphyrinogens, a few mols. of which were previously known, but not recognized as possessing anion- or mol.-binding properties. The binding mode is noncovalent, primarily that of hydrogen-bonding, thereby providing a new mode for liq. chromatog., that of hydrogen bonding liq. chromatog. Further useful applications of the macrocycles include environmental remediation by removal of undesired ions or neutral mols., and removal of phosphate for kidney dialysis. Thus, calix[4]pyrrole I was prep. by cyclization of pyrrole and acetone in the presence of MeSO3H, which was added slowly to prevent a violent reaction. II was prep. by reaction of pyrrole with cyclohexanone in the presence of HCl. Stability consts. for I and II were detd. to demonstrate their affinity for various ions in soln., e.g. giving a const. of 350 ± 5.5 M-1 for chloride.

IT 190517-33-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); NNU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of calixpyrroles, calixpyridinopyrroles and calixpyridines)  
 RN 190517-33-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9Cl) (CA INDEX NAME)

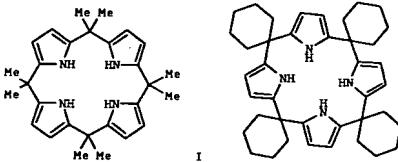


L6 ANSWER 89 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1997:684406 CAPLUS  
 DOCUMENT NUMBER: 127:346236  
 TITLE: preparation of calixpyrroles, calixpyridinopyrroles and calixpyridines  
 INVENTOR(S): Gale, Philip A.; Sessler, Jonathan L.; Genge, John W.; Kral, Vladimir; Andrievsky, Andrei; Lynch, Vincent; Samon, Petra I.; Allen, William E.; et al.  
 PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA  
 SOURCE: PCT Int. Appl., 145 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9737995	A1	1997/01/06	WO 1997-05643	1997/04/04
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BE, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG	AA	1997/01/06	CA 1997-2251072	1997/04/04
CA 2251072	AA	1997/01/06	CA 1997-2251072	1997/04/04
CA 2391030	AA	1997/01/06	CA 1997-2391030	1997/04/04
AU 9724409	A1	1997/10/29	AU 1997-24409	1997/04/04
EP 891364	A1	1999/01/20	EP 1997-920143	1997/04/04
R: CH, DE, FR, GB, IT, LI, NL, SE				
JP 2000511880	T2	2000/09/12	JP 1997-536364	1997/04/04
PRIORITY AFFIN. INFO.:			US 1996-14890P	P 1996/04/05
			US 1996-24203P	P 1996/08/27
			US 1996-26694P	P 1996/09/25
			US 1996-33395P	P 1996/12/17
			US 1996-33396P	P 1996/12/17
			CA 1997-2251072	A3 1997/04/04
			WO 1997-05643	W 1997/04/04

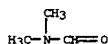
OTHER SOURCE(S): MARPAT 127:346236

GI



AB Preparation of calixpyrrole, calixpyridinopyrrole, and calixpyridine macrocycles having 4, 5, 6, 7, or 8 heterocyclic rings, such as I and II,



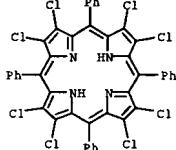


IT 120644-25-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, UV-visible spectrum and complexation with terbium)

RN 120644-25-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

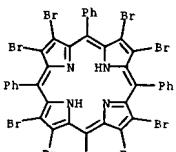


IT 131214-86-3P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, mol. structure, UV-visible spectrum and complexation with terbium)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 92 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1997:318649 CAPLUS  
DOCUMENT NUMBER: 127:4955

TITLE: Syntheses and structural properties of severely distorted porphyrins: N-methyl derivatives

AUTHOR(S): Clement, Todd E.; Nguyen, Liem T.; Khouri, Richard G.; Nurco, Daniel J.; Smith, Kevin M.

CORPORATE SOURCE: Dep. Chemistry, Univ. California, Davis, CA, 95616, USA

SOURCE: Heterocycles (1997), 45(4), 651-658

CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

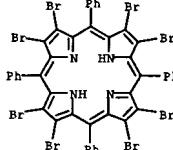
AB Syntheses and characterization of a series of N-methylated derivs. of sterically distorted porphyrins are reported; the work includes the first example of a tetra-N-methylated porphyrin obtained by methylation of an intact porphyrin.

IT 131214-86-3

RL: RCT (Reactant); RACT (Reactant or reagent) (syntheses and structural properties of severely distorted N-methylporphyrins)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

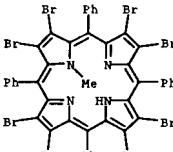


IT 190382-01-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (syntheses and structural properties of severely distorted N-methylporphyrins)

RN 190382-01-5 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-21-methyl-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 93 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:275704 CAPLUS

DOCUMENT NUMBER: 127:17652

TITLE: Calix[4]pyrroles: C-rim substitution and tunability of anion binding strength

AUTHOR(S): Gale, Philip A.; Sessler, Jonathan L.; Allen, William E.; Tvermoe, Nicolai A.; Lynch, Vincent

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University

of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Chemical Communications (Cambridge) (1997), (7), 665-666

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Electron-rich and electron-deficient C-rim substituted calix[4]pyrroles are synthesized and the anion binding ability of these receptors is found to be dependent upon the C-rim substituents.

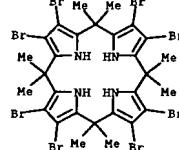
IT 190517-33-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and tunability of anion binding strength of calixpyrroles)

RN 190517-33-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)

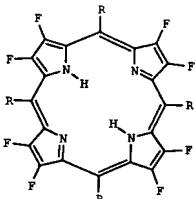


REFERENCE COUNT:

14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 94 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1997180900 CAPLUS

DOCUMENT NUMBER: 126157325  
TITLE: 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetraarylporphyrins and Their Zinc Complexes: First Spectroscopic, Electrochemical, and Structural Characterization of a Perfluorinated Tetraarylmetalloporphyrin  
AUTHOR(S): Woller, Eric K.; DiMaggio, Stephen G.  
CORPORATE SOURCE: Department of Chemistry, University of Nebraska, Lincoln, NE, 68588-0304, USA  
SOURCE: Journal of Organic Chemistry (1997), 62(6), 1588-1593  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



I

AB A convenient and general synthesis of  $\beta$ -octafluoroporphyrins I [R = Ph, C6F5, 3-MeC6H4] is reported. The structural, spectroscopic, and electrochem. data indicate that  $\beta$ -octafluoro-meso-tetraarylporphyrins are a new class of planar, electron-deficient ligands. Particularly impressive is the 0.5 V window over which the formal oxidation potential can be tuned using only aryl substituents. The invariance of the ligand structure with increasingly pos. formal oxidation potential is a key advance;

electronic effects have been severed from the nonplanar conformations exhibited by all other highly electron-deficient porphyrins.

IT 121399-88-0P 186885-28-9P

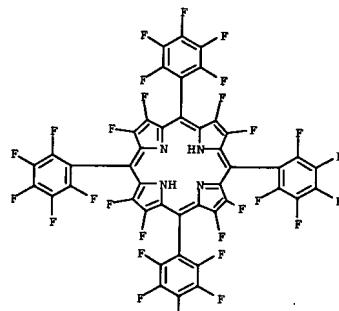
RL: PFP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and characterization of octafluorotetraarylporphyrins)

RN 121399-88-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

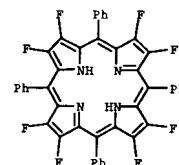
L6 ANSWER 94 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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RN 186885-28-9 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



IT 186885-29-0P

RL: PFP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and characterization of octafluorotetraarylporphyrins)

RN 186885-29-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 94 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

ACCESSION NUMBER: 1996703905 CAPLUS  
DOCUMENT NUMBER: 126181682  
TITLE: Nonlinear absorption in modified porphyrins  
AUTHOR(S): Tang, N.; Su, W.; Cooper, T.; Adams, W.; Brandelik, D.; Brant, M.; McLean, D.; Sutherland, R.  
CORPORATE SOURCE: Wright Lab, WL/MLPJ, WPAFB, OH, 45433, USA  
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1996), 2853(Nonlinear Optical Liquids), 149-157  
PUBLISHER: SPIE-The International Society for Optical Engineering  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The authors study one free base and seven metallo-octabromotetraphenylporphyrins by several techniques. In a pico-second pump-probe experiment, the authors monitor the transient transmission of each

sample up to 11 ns after it is irradiated by an intense laser pulse. Combined with the results from time-resolved fluorescence spectroscopy, the authors propose a simple model to interpret the transmission data. The authors attribute the reduction in the transmission to triplet state absorption and extract the triplet state absorption cross sections, as well as the lifetimes from the time dependent transmission data. In a sep. experiment where the transmission of a nanosecond laser pulse is measured with

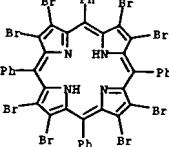
various input energies, the authors' measurement in the cross sections predicts the correct optical limiting behavior. The authors assess the overall optical limiting performance of all 8 samples by direct comparison with C60 at the same ground state transmission.

IT 131214-86-3

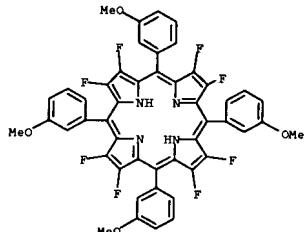
RL: PFP (Properties) (nonlinear absorption and optical limiting for modified porphyrins)

RN 131214-86-3 CAPLUS

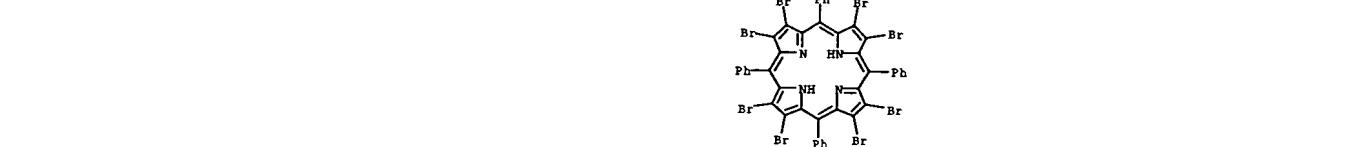
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



L6 ANSWER 94 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



L6 ANSWER 96 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1996:680693 CAPLUS  
 DOCUMENT NUMBER: 126167289  
 TITLE: Photocatalytic oxidation of cyclohexane by (nBu4N)4W10032/Fe(III)porphyrins integrated systems  
 AUTHOR(S): Maldotti, Andrea; Molinari, Alessandra; Bergamini, Paola; Amadelli, Rossano; Battioni, Pierrette; Mansuy, Daniel  
 CORPORATE SOURCE: Dipartimento di Chimica, Centro di Studio su Fotocatalisi e Catalisi del CNR, Universita degli Studi di Ferrara, Via L. Borsari 46, Ferrara, 44100, Italy  
 SOURCE: Journal of Molecular Catalysis A: Chemical (1996), 113(1-2), 147-157  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The oxidation of cyclohexane by photoexcited (nBu4N)4W10032 has been investigated in the presence of iron meso-tetraarylporphyrins bearing different substituents in the  $\beta$ -pyrrole positions and/or in the meso-aryl groups. Irradiation at 325 nm leads to the reduction of the polyoxotungstate with the simultaneous oxidation of cyclohexane to cyclohexyl radicals which can be detected by the ESR spin trapping technique. In oxygen-free solns., the photoreduced polyoxotungstate is able to transfer one electron to the Fe(III)porphyrin to give the ferrous complex. The subsequent reaction between this species and cyclohexyl radicals leads to the formation of  $\alpha$ -alkyl-Fe(III)porphyrin complexes, as demonstrated by UV-visible and NMR spectroscopy. In the presence of oxygen, the photoreduced polyoxotungstate has the role of initiating the activation of O<sub>2</sub> through its reduction to O<sub>2</sub><sup>•-</sup> and H<sub>2</sub>O<sub>2</sub>. As a consequence, cyclohexane is converted to cyclohexanone and cyclohexanol in a cyclic way. The Fe(III)porphyrin complex strongly affects the product distribution probably through its hydrogen peroxide and alkyl-hydroperoxide-dependent oxidation. In comparison with (nBu4N)4W10032 alone, a higher selectivity is obtained with the formation of cyclohexanol as major product.

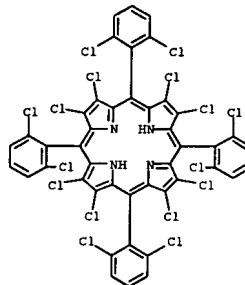
IT 134833-67-3D, iron complexes

RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses); (photocatalytic property of polyoxotungstate/iron tetraarylporphyrin system for oxidation of cyclohexane)

RN 134833-67-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 96 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 97 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1996:674168 CAPLUS  
 DOCUMENT NUMBER: 125315678  
 TITLE: Gas reactive pigment, gas detector using the same, and gas detection method and apparatus using the detector  
 INVENTOR(S): Tanaka, Kazuharu; Igarashi, Chiaki; Sadaoka, Yoshihiko  
 PATENT ASSIGNEE(S): Ebara Corporation, Japan; Ebara Research Co., Ltd.  
 SOURCE: Eur. Pat. Appl., 31 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 733901	A2	1996025	EP 1996-104433	19960320
EP 733901	A3	19961211		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 09171011	A2	19970630	JP 1996-50431	19960307
TW 464651	B	20011121	TW 1996-85104567	19960417
PRIORITY APPLN. INFO.:			JP 1995-85988	A 19950320
			JP 1995-270139	A 19951018
			JP 1996-50431	A 19960307

OTHER SOURCE(S): MARPAT 125:315678

AB A gas reactive pigment reactive to at least one of a halogen gas, a hydrogen halide gas, an acidic gas, an oxidizing gas, a basic gas, and an organic acid gas is provided. The pigment comprises a metal complex of tetraphenylporphyrin or a derivative thereof (I) wherein M represents a transition metal; a plurality of R's independently represent a hydrogen atom, a halogen atom, a nitro group, a cyano group or an alkoxy group, or a tetraphenylporphyrin derivative (II) wherein a plurality of R's independently represent a hydrogen atom, a halogen atom, a nitro group, a cyano group or an alkoxy group; a plurality of G's on the 4 Ph groups all represent a substituent selected from a halogen atom, a hydroxyl group, a sulfonic acid group, a carboxyl group, an alkoxy group, and an amino group, the positions of which on the 4 Ph groups may be the same or different; and a, b, c and d which may be the same or different, each represents an integer of 0 to 5, indicating the number of G's on each Ph group; provided that the compound wherein all R's represent a hydrogen atom, and a, b, c and d all represent 0 is excluded. A detector for the above gases containing the reactive pigment; a method for detecting the above

gases

using the detector; and a detection apparatus for the above gases using the detector are also provided. The gas reactive pigment shows a color change, which can be measured in terms of the absorption spectrum change of said pigment at high sensitivity on contact with the above gases.

IT 131214-86-3, 2, 3, 7, 8, 12, 13, 17, 18-Octabromo-5,10,15,20-tetraphenylporphyrin

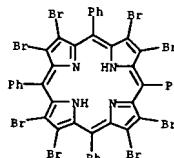
RL: ARG (Analytical reagent use); DEV (Device component use); ANST (Analytical study); USES (Uses)

(gas anal. by detector based on tetraphenylporphyrin metal complexes)

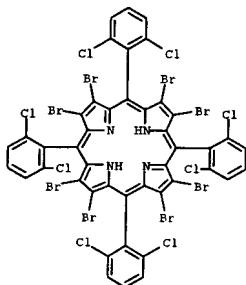
RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 97 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

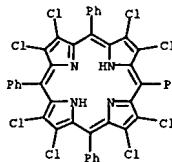


L6 ANSWER 98 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1996673496 CAPLUS  
 DOCUMENT NUMBER: 125:346125  
 TITLE: Porphyrins bearing halogens at the meso-phenyl and  $\beta$ -pyrrolic positions: synthesis and spectral properties  
 AUTHOR(S): Wijesekera, Tilak; Dupre, Daniel; Cader, Mohamed S. R.; Dolphin, David  
 CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Z1, Can.  
 SOURCE: Bulletin de la Societe Chimique de France (1996), 133(7-8), 765-775  
 CODEN: BSCFAS; ISSN: 0037-8968  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The synthesis of sym. porphyrins chlorinated at both ortho positions of the meso-aryl substituents, and the chlorination and bromination of the  $\beta$ -pyrrole positions is reported. The  $\beta$ -chlorination of meso-tetraphenylporphyrin via its nickel(II) complex is also described. The authors communicate the 1st perchlorination of tetramesitylporphyrin, where halogen substitution occurred at the  $\beta$ -pyrrolic positions as well as at both the vacant meta positions of the trimethylphenyl groups. The iron complexes of these various polyhalogenated porphyrins are also described, since they are robust and efficient catalysts in oxidation reactions.  
 IT 107035-95-OP 120644-25-9P 131214-86-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and complexation with iron)  
 RN 107035-95-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

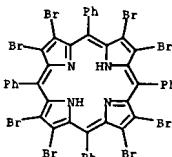


RN 120644-25-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 98 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

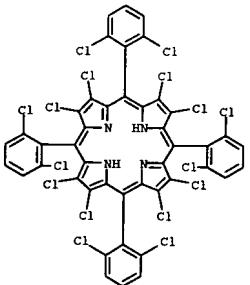


RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



IT 134833-67-3P 183594-03-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 134833-67-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

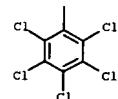
L6 ANSWER 98 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



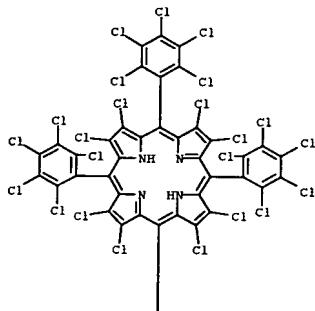
RN 183594-03-8 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentachlorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 98 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

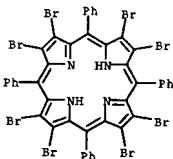
PAGE 2-A



PAGE 1-A

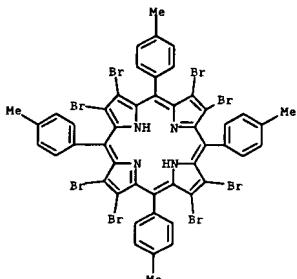


L6 ANSWER 99 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1996:1552458 CAPLUS  
 DOCUMENT NUMBER: 125:291504  
 TITLE: *meso*-Substituted octabromoporphyrins: synthesis, spectroscopy, electrochemistry and electronic structure  
 AUTHOR(S): Hariprasad, Gali; Dahal, Sanjay; Maiya, Bhaskar G.  
 CORPORATE SOURCE: School Chemistry, University Hyderabad, Hyderabad, 500 046, India  
 SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1996), (16), 3429-3436  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The free-base, copper(II) and zinc(II) derivs. of 5,10,15,20-tetraarylporphyrin (aryl = Ph, 4-methylphenyl or 4-chlorophenyl) and the corresponding brominated 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraarylporphyrin derivs. were synthesized and their spectral and redox properties compared by UV-visible, <sup>1</sup>H NMR, ESR, and cyclic voltammetric methods. Substitution with the electron-withdrawing bromine groups at the pyrrole carbons has a profound influence on the UV-visible and <sup>1</sup>H NMR spectral features and also on the redox potentials of these systems. However, electron-withdrawing chloro or electron-donating Me groups at the para positions of the four Ph rings have only a marginal effect on the spectra and redox potentials of both the brominated and the nonbrominated derivs. The ESR data for the copper(II) derivs. of all these systems reveal that substitution at either the  $\beta$ -pyrrole carbons and/or the para positions of the *meso*-Ph groups does not significantly affect the spin-Hamiltonian parameters that describe the metal center in each case. Collectively, these observations suggest that the highest-occupied (HOMO) and lowest-unoccupied MOs (LUMO) of the octabromoporphyrins involve the porphyrin  $\pi$ -ring system as is the case with the nonbrominated derivs. Studies were carried out to probe the electronic structures of these systems by three different approaches involving spectral and redox potential data as well as AM1 calcns. The electron-withdrawing  $\beta$ -bromine substituents stabilize the LUMOs and, to a lesser degree, the HOMOs and the extent of these changes can be fine-tuned, in a subtle way, by substitution on the *meso*-aryl rings of a given porphyrin.  
 IT 131214-86-3  
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
 (electronic structure and electrochem. redox of)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetr phenyl- (9CI) (CA INDEX NAME)

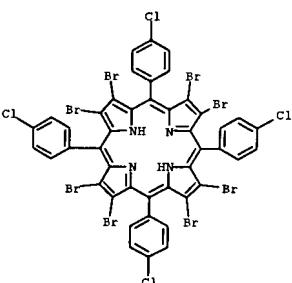


IT 182423-35-4P 182423-39-8P

L6 ANSWER 99 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn., complexation with copper or zinc, electronic structure and electrochem. redox of)  
 RN 182423-35-4 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-methylphenyl)- (9CI) (CA INDEX NAME)



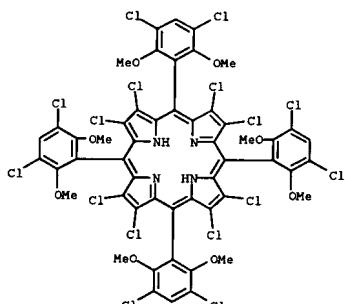
RN 182423-39-8 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-chlorophenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 100 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1996:422809 CAPLUS  
 DOCUMENT NUMBER: 125:179700  
 TITLE: Synthesis and electrochemistry of 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)porphyrin (H<sub>2</sub>tdcdmpp) [CoII(tcdmpp)] and [M(tcdmpp)Cl] (M = FeIII or MnIII)  
 AUTHOR(S): Autret, Marie; Gu, Zhongping; Antonini, Alessandra; Boschi, Tristano; Tagliatela, Peitro; Kadish, Karl M.  
 CORPORATE SOURCE: Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA  
 SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1996), (13), 2793-2797  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Four new highly chlorinated porphyrins, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)porphyrin (H<sub>2</sub>tdcdmpp) and [M(tcdmpp)Cl] (M = FeIII or MnIII) were prepared. The free base was synthesized by chlorination of H<sub>2</sub>tdmmp [5,10,15,20-tetrakis(2,6-dimethoxyphenyl)porphyrin] and metalated to give the complexes following published procedures. The same transition-metal derivs. of tdmpp were also prepared and all eight synthesized compds. were electrochem. studied in benzene/tetrakis(1,10-phenanthroline) containing 0.1 mol dm<sup>-3</sup> NBu<sub>4</sub>ClO<sub>4</sub>. As expected the half-wave potentials of the tcdmpp complexes are shifted towards pos. values while those for oxidation or reduction of the tdmpp species are shifted neg. as compared with E<sub>1/2</sub> for oxidation or reduction of tetraphenylporphyrin (tpy) complexes having the same central metal ions. The magnitude of the anodic shifts in E<sub>1/2</sub> for reduction with respect to tpy is among the largest reported for chlorinated porphyrins and ranges between 590 and 860 mV depending upon the specific redox reaction and solvent. A smaller AE<sub>1/2</sub> of 330-400 mV is seen for oxidation of the same compds. and these values can be compared to a negligible shift in E<sub>1/2</sub> upon going from planar M(tpy) to distorted M(obtpy) (obtpy = 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetr phenylporphyrinate) complexes of cobalt and iron where the effect of macrocycle ruffling is known to predominate over the electronic effects of added halide substituents. The core distortion cannot compensate totally for the electron-withdrawing effect of the Cl substituents. The macrocyclic distortion also induces a large red shift of the UV-visible absorption bands and this shift in A<sub>max</sub> ranges up to 40 nm for the chlorinated compds. with respect to the tdmpp complexes.

IT 180711-85-7P, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)porphyrin  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction with transition metal salts and elec. oxidation and reduction potentials of)  
 RN 180711-85-7 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 100 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

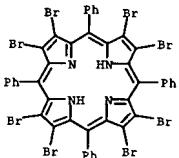


AB The core distortion cannot compensate totally for the electron-withdrawing effect of the Cl substituents. The macrocyclic distortion also induces a large red shift of the UV-visible absorption bands and this shift in A<sub>max</sub> ranges up to 40 nm for the chlorinated compds. with respect to the tdmpp complexes.

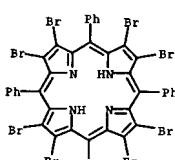
IT 180711-85-7P, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dimethoxyphenyl)porphyrin  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction with transition metal salts and elec. oxidation and reduction potentials of)  
 RN 180711-85-7 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

Chemical structure of a meso-substituted octachloroporphyrin with 3,5-dimethoxyphenyl groups at the meso-positions. The structure is identical to the one above, except the para-positions of the four phenyl rings are replaced by 3,5-dimethoxyphenyl groups.

L6 ANSWER 101 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1996:396653 CAPLUS  
 DOCUMENT NUMBER: 125:195272  
 TITLE: Manifestation of structural features of porphyrin molecules in their electron absorption spectra  
 AUTHOR(S): Berezin, D. B.; Andriyanov, V. G.; Semeikin, A. S.  
 CORPORATE SOURCE: Ivanovskaya Gosudarstvennaya Khimiko-Tekhnologicheskaya Akademiya, Ivanovo, 153460, Russia  
 SOURCE: Optika i Spektroskopiya (1996), 80(4), 618-626  
 CODEN: OFSPAM; ISSN: 0030-4034  
 PUBLISHER: MAIK Nauka  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB The suggested earlier hypothesis on the nature of the intense absorption band at 350-450 nm is discussed. This band may be caused by photoinduced transfer of the electron d<sub>4</sub> from the pyrrole rings to the macrocyclic system. For porphyrins and their aza derivs. the information available from the value of the long-wave absorption band shift under protonation of the compds. is analyzed.  
 IT 131214-86-3P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and electronic structure of porphyrins by UV)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-(9Cl) (CA INDEX NAME)



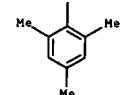
L6 ANSWER 102 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1996:306509 CAPLUS  
 DOCUMENT NUMBER: 125:25070  
 TITLE: Optochemical HCl and Cl<sub>2</sub> gas detection based on tetraphenylporphine dispersed in ethyl-cellulose  
 AUTHOR(S): Tagliatesta, Pietro; Sadaoka, Yoshihiko; Sakai, Yoshiro  
 CORPORATE SOURCE: Dip. Sci. Tecnologie Chim., Univ. degli Roma, Tor Vergata, 00173, Italy  
 SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1996), 278, 173-180  
 CODEN: MCLCE9; ISSN: 1058-725X  
 PUBLISHER: Gordon & Breach  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB To detect sub-ppm levels of HCl gas, spectral changes of tetraphenylporphine and derivs. dispersed in ethylcellulose were examined in the visible region. For free base tetraphenylporphyrin, the absorbance at 450 nm and 670 nm is sensitive to sub-ppm levels of HCl and also a good reversibility is observed at room temperature. The Soret and Q-bands are insensitive to NH<sub>3</sub>, Cl<sub>2</sub>, NO<sub>2</sub> and NO at room temperature. For zinc tetra(bromotetraphenylporphine), the absorbance at 479 nm and 722 nm is sensitive to sub-ppm levels of HCl gas and also good reversibility is observed at room temperature.  
 IT 131214-86-3  
 RL: PRP (Properties) (Visible spectrum of)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-(9Cl) (CA INDEX NAME)



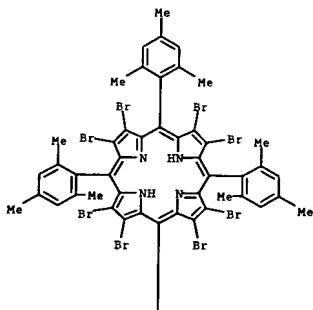
L6 ANSWER 103 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1996:290273 CAPLUS  
 DOCUMENT NUMBER: 124:342946  
 TITLE: Synthesis of  $\beta$ -Mono-, Tetra-, and Octasubstituted Sterically Bulky Porphyrins via Suzuki Cross Coupling  
 AUTHOR(S): Zhou, Xiang; Tse, Man Kin; Wan, Terence S. M.; Chan, Kin Shing  
 CORPORATE SOURCE: Departments of Chemistry, Chinese University of Hong Kong, Shatin, Hong Kong  
 SOURCE: Journal of Organic Chemistry (1996), 61(11), 3590-3593  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB  $\beta$ -Mono-, tetra-, and octa-substituted tetramesitylporphyrins were prepared in good yields by Suzuki cross-coupling reactions of  $\beta$ -bromotetramesitylporphyrins with aryl- and alkylboronic acids.  
 IT 129006-48-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis of sterically bulky porphyrins via Suzuki cross-coupling reactions)  
 RN 129006-48-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-(9Cl) (CA INDEX NAME)

L6 ANSWER 103 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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PAGE 1-A



ACCESSION NUMBER: 1996:271551 CAPLUS  
 DOCUMENT NUMBER: 124:316876  
 TITLE: Haloporphyrins and their preparation  
 INVENTOR(S): Ellis, Paul E., Jr.; Lyons, James E.  
 PATENT ASSIGNEE(S): Sun Company, Inc. (Rm), USA  
 SOURCE: Eur. Pat. Appl., 8 pp.  
 CODEN: EPKNDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 11  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 700915	A1	19960313	EP 1995-306230	19950906
R: BE, DE, FR, GB, IT, NL				
CA 2157241	AA	19960308	CA 1995-2157241	19950830
JP 08113575	A2	19960507	JP 1995-254492	19950907
US 5663328	A	19970902	US 1996-672202	19960627
PRIORITY APPLN. INFO.:				
US 1994-303106	A	19940907		
US 1987-246	A2	19870102		
US 1987-66666	A2	19870626		
US 1989-425089	B2	19891023		
US 1990-568116	A2	19900816		

OTHER SOURCE(S): MARPAT 124:316876

AB The invention provides novel catalyst compns., useful in the oxidation of hydrocarbons with air or oxygen to form hydroxy-group containing compds. and in the decomposition of hydroperoxides to form hydroxy-group containing compds.

The catalysts comprise transition metal complexes of a porphyrin ring having 1 to 12 halogen substituents on the porphyrin ring, at least one of said halogens being in a meso position and/or the catalyst containing no aryl

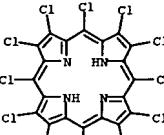
group in a meso position. The compns. are prepared by halogenating a transition metal complex of a porphyrin. Thus, Cu porphyrin was chlorinated with Cl in CCl<sub>4</sub> to give the dodecachloroderiv. which was demetalated and then remetalated to give iron meso-tetrachloro-8-octachloroporphyrin chloride (I). I was used as a catalyst in the oxidation of isobutane to give mainly Me<sub>3</sub>COH and in the decomposition of Me<sub>3</sub>COOH to MeCOH.

IT 144811-82-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of perhaloporphyrin complexes as oxidation catalysts)

RN 144811-82-5 CAPLUS

CN 21H,23H-Porphine, 2,3,5,7,8,10,12,13,15,17,18,20-dodecachloro- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1996:247527 CAPLUS

DOCUMENT NUMBER: 124:342944

TITLE: En route to 2,3,7,8,12,13,17,18-octafluoroporphyrin

AUTHOR(S): Leroy, Jacques

CORPORATE SOURCE: Ec. Normale Supérieure, Dep. Chimie, Paris, 75231, Fr.

SOURCE: Electronic Conference on Trends in Organic Chemistry

[CD-ROM] (1996), Meeting Date 1995, Paper 40

Editor(s): Rzepa, Henry S.; Leach, Christopher;

Goodman, Jonathan M. Royal Society of Chemistry:

Cambridge, UK.

CODEN: 62TKAB

DOCUMENT TYPE: Conference

LANGUAGE: English

AB A symposium report with 13 refs. on the preparation of fluoropyrrole intermediates for octafluoroporphyrin.

IT 144811-86-9P

RL: PNU (Preparation, unclassified); PREP (Preparation); (preparation of intermediates for octafluoroporphyrin)

RN 144811-86-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)

ACCESSION NUMBER: 1996:182893 CAPLUS

DOCUMENT NUMBER: 124:300066

TITLE: Metalation of water-soluble octabromoporphyrin with lithium(I), cadmium(II), and mercury(II)

AUTHOR(S): Tabata, Masaaki; Nishimoto, Jun; Ogata, Akiko; Kusano, Tohru; Nahar, Nurur

CORPORATE SOURCE: Dep. Chemistry, Saga Univ., Saga, 840, Japan

SOURCE: Bulletin of the Chemical Society of Japan (1996),

69(3), 673-77

CODEN: BCJSJA; ISSN: 0009-2673

PUBLISHER: Nippon Kagakkai

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A water soluble porphyrin, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin (H<sub>2</sub>obtpp4-, H<sub>2</sub>P4-) was synthesized and the equilibrium consts. were determined for the reaction of H<sub>2</sub>obtpp4-

with Li<sup>+</sup>,Cd<sup>2+</sup>, and Hg<sup>2+</sup> at 25° in I = 0.1 mol dm<sup>-3</sup> (NaNO<sub>3</sub>). The protonationconsts. of H<sub>2</sub>obtpp4- were determined. The porphyrin reacted with Li<sup>+</sup> in

alkaline aqueous solution to form LiP5-, for which formation constant was determined

Na and K ions did not form their complexes under the same exptl. conditions. The equilibrium consts. for the formation of Cd<sup>2+</sup> and Hg<sup>2+</sup> porphyrins were determined. Hg<sup>2+</sup> also forms homodinuclear porphyrin, Hg<sub>2</sub>P for which the formation constant was determined. The octabromo groups lower the basicityof the porphyrin, which gave Li<sup>+</sup> porphyrin.

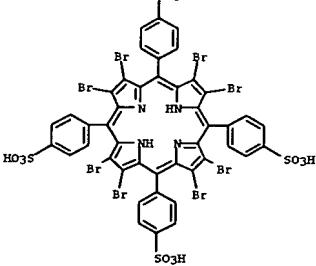
IT 154783-99-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(complexation with cadmium and mercury and lithium)

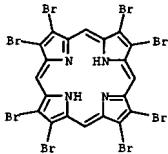
RN 154783-99-0 CAPLUS

CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis- (9CI) (CA INDEX NAME)

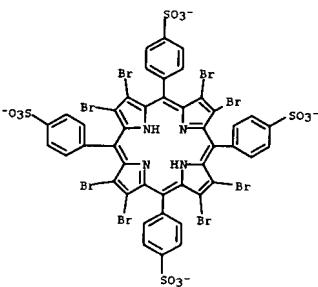


RL: PNU (Formation, unclassified); PRP (Properties); FORM (Formation,

L6 ANSWER 106 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 nonpreparative)  
 (formation consts.  
 IT 144811-83-6P, 2,3,7,8,12,13,17,18-Octabromoporphyrin  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and sulfonation of)  
 RN 144811-83-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



IT 176173-80-1  
 RL: PRP (Properties)  
 (protonation consts.)  
 RN 176173-80-1 CAPLUS  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis-, ion(4-) (9CI) (CA INDEX NAME)



L6 ANSWER 107 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 1996:161613 CAPLUS  
 124:316505  
 TITLE: Partial oxidation of hydrocarbons and decomposition of hydroperoxides catalyzed by haloporphyrin metal complexes  
 INVENTOR(S): Ellis, Paul E., Jr.; Lyons, James E.  
 PATENT ASSIGNEE(S): Sun Co., Inc. (R and M), USA  
 SOURCE: U.S., 5 pp. Cont.-in-part of U.S. Ser. No. 568,116.  
 CODEN: USXXAM

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 11  
 PATENT INFORMATION:

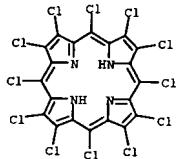
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5489716	A	19960206	US 1994-303105	19940907
US 4955682	A	19900123	US 1987-246	19870102
US 4900871	A	19900213	US 1987-66666	19870626
CA 1336188	A1	19950704	CA 1987-553420	19871203
US 5093491	A	19920303	US 1990-466163	19900117
CA 2157238	AA	19960308	CA 1995-2157238	19950830
EP 704447	A1	19960403	EP 1995-306231	19950906
R: BE, DE, FR, GB, IT, NL				
JP 08104658	A2	19960423	JP 1995-254493	19950907
US 5663328	A	19970902	US 1996-672202	19960627
PRIORITY APPLN. INFO.:				
		US 1987-246	A2	19870102
		US 1987-66666	A2	19870626
		US 1990-568116	A2	19900816
		US 1989-425089	B2	19891023
		US 1994-303105	A	19940907
		US 1994-303106	A3	19940907

OTHER SOURCE(S): CASREACT 124:316505; MARPAT 124:316505  
 AB The invention provides novel methods for the oxidation of hydrocarbons with oxygen-containing gas to form hydroxy-group containing compds. and for the decomposition of hydroperoxides to form hydroxy-group containing compds.

The catalysts used in the methods of the invention comprise transition metal complexes of a porphyrin ring having 1 to 12 halogen substituents on the porphyrin ring, at least one of said halogens being in a meso position and/or the catalyst containing no aryl group in a meso position. The catalyst compns. are prepared by halogenating a transition metal complex of a porphyrin. In one embodiment, a complex of a porphyrin with a metal whose porphyrin complexes are not active for oxidation of alkanes is halogenated, thereby to obtain a haloporphyrin complex of that metal, the metal is removed from the haloporphyrin complex to obtain the free base form of the haloporphyrin, and a metal such as iron whose porphyrin complexes are active for oxidation of alkanes and for the decomposition of alkyl hydroperoxides is complexed with the free base to obtain an active catalyst for oxidation of alkanes and decomposition of alkyl hydroperoxides. Thus, partial oxidation product.

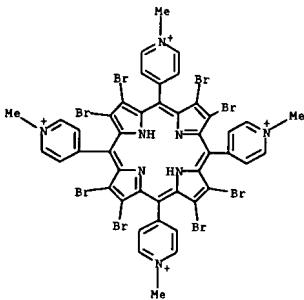
Decomposition of tert-Bu hydroperoxide in tert-Bu alc. catalyzed by iron complex of meso-tetrachloro- $\beta$ -octachloroporphyrin afforded tert-Bu alc.

L6 ANSWER 107 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 IT 144811-82-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (partial oxidation of hydrocarbons and decomposition of hydroperoxides catalyzed by haloporphyrin metal complexes)  
 RN 144811-82-5 CAPLUS  
 CN 21H,23H-Porphine, 2,3,5,7,8,10,12,13,15,17,18,20-dodecachloro- (9CI) (CA INDEX NAME)



L6 ANSWER 108 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 1996:145243 CAPLUS  
 124:213140  
 TITLE: Observation of a Stable Water-Soluble Lithium Porphyrin  
 AUTHOR(S): Richards, Rosalie A.; Hammons, Kelly; Joe, Melanie; Miskelly, Gordon M.  
 CORPORATE SOURCE: Department of Chemistry, University of Southern California, Los Angeles, CA, 90089-0744, USA  
 SOURCE: Inorganic Chemistry (1996), 35(7), 1940-4  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The deprotonated form of the water soluble porphyrin 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(N-methylpyridinium-4-yl)porphyrin, H<sub>2</sub>OBT(4-N-MePy)P4+, has a strong affinity for Li<sup>+</sup> and forms a stable Li complex in basic aqueous solution. The fully deprotonated form, OBT(4-N-MePy)P2+, is present above pH 10 (pKa3 = 6.5 ± 0.1 and pKa4 = 10.2 ± 0.1). Li ions bind to this porphyrin in aqueous solution in a 1:1 stoichiometry with a binding constant of (9.6 ± 0.5) + 102 M<sup>-1</sup> (0.1M KOH, 298 K). The apparent binding constant for Li<sup>+</sup> is reduced in the presence of a large excess of Na<sup>+</sup>, and a binding constant for Na<sup>+</sup> of 1.0 ± 0.3M<sup>-1</sup> was obtained. The Li<sup>+</sup> porphyrin in D<sub>2</sub>O shows a <sup>7</sup>Li NMR signal at -10.25 ppm vs. 1.1M LiCl, and the line widths show exchange occurs at 299 K, in contrast to earlier Li porphyrins, which exchange more slowly. The Li-binding behavior and <sup>7</sup>Li NMR spectra for 5,10,15,20-tetrakis(N-methylpyridinium-4-yl)porphyrin, H<sub>2</sub>M(4-N-MePy)P(2+x)+ (x = 0-2) are also reported.

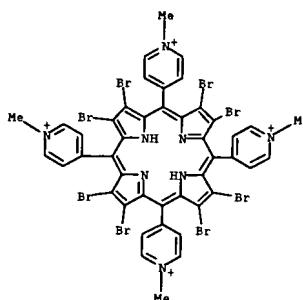
IT 174580-25-7P 174580-27-9P  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (preparation and binding consts. with lithium)  
 RN 174580-25-7 CAPLUS  
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[1-methyl- (9CI) (CA INDEX NAME)



RN 174580-27-9 CAPLUS  
CN Pyridinium, 4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[1-methyl-, tetrakis(hexafluorophosphate(1-)), mono(hexafluorophosphate(1-)) (9CI) (CA INDEX NAME)

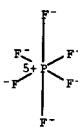
CM 1

CRN 16940-81-1  
CMF F6 P . H  
CCI CCS



CH 4

CRN 16919-18-9  
CMF F6 P  
CCI CCS



IT 174580-33-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 174580-33-7 CAPLUS  
CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[1-methyl-, tetrachloride (9CI) (CA INDEX NAME)

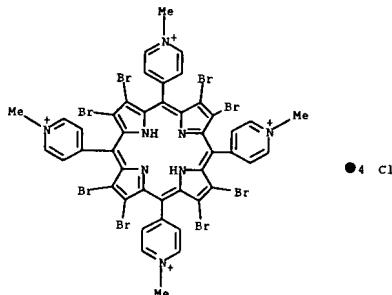
● H<sup>+</sup>

CM 2

CRN 174580-26-8  
CMF C44 H30 Br8 N8 . 4 F6 P

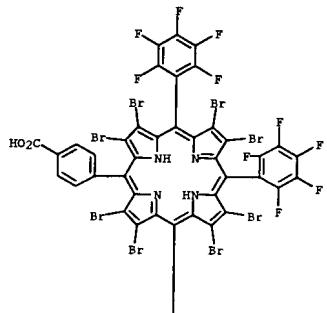
CM 3

CRN 174580-25-7

● 4 Cl<sup>-</sup>

L6 ANSWER 109 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1996:25316 CAPLUS  
DOCUMENT NUMBER: 124:101510  
TITLE: Energy Transfer and Electron Transfer of Poly(ethylene glycol)-Linked Fluorinated Porphyrin Derivatives in Lipid Bilayers  
AUTHOR(S): Nango, Mamoru; Iida, Kouji; Matsuura, Mitsutaka; Yamaguchi, Masashi; Sato, Kiyohito; Tanaka, Kazumasa; Akimoto, Kyoko; Yamashita, Keiji; Tsuda, Kazuichi; Kurono, Yukihisa  
CORPORATE SOURCE: Department of Applied Chemistry, Nagoya Institute of Technology, Nagoya, 466, Japan  
SOURCE: Langmuir (1996), 12(2), 450-8  
PUBLISHER: CODEN: LANGD5; ISSN: 0743-7463  
DOCUMENT TYPE: American Chemical Society  
LANGUAGE: English  
AB Poly(ethylene glycol) [PEG]-linked porphyrin derivs. separated by spacer methylene groups (C<sub>n</sub>), PEG-C<sub>n</sub>-MnPPFP (M = H<sub>2</sub>, Mn; n = 0, 5, 11), PEG-C11-MnTP (M = H<sub>2</sub>, Mn), and PEG-CO-MnPPFP (M = H<sub>2</sub>, Mn) were synthesized. The porphyrin portion of the poly(ethylene glycol) [PEG]-linked fluorinated porphyrin derivative has been anchored onto a lipid bilayer. PEG-linked fluorinated porphyrins easily associated with phospholipid bilayers and are chemical stable against oxidants such as H<sub>2</sub>O<sub>2</sub>. An efficient energy transfer from phospholipid-linked zinc porphyrin, PE-C11-ZnPPFP, to externally added PEG-C<sub>n</sub>-H2PPFP (n = 0, 5, 11) in the lipid bilayer was observed, depending on the length of C<sub>n</sub> and the porphyrin structure. Ground state transmembrane electron transfer catalyzed by PEG-Cn-MnPPFP (n = 0, 5, 11) and PEG-C11-MnTP revealed that the porphyrin causes a significant accelerated electron transfer especially when n = 11. Comparison of PEG-C11-MnPPFP- and PEG-C11-MnTP-catalyzed electron transfer is made. The electron transfer rate was controlled not only by the separated spacer methylene groups between the porphyrin and PEG moieties but also by the structures of porphyrins.  
IT 172663-37-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(in preparation of polyethylene glycol-linked fluorinated porphyrin derivs.)  
RN 172663-37-5 CAPLUS  
CN Benzoic acid, 4-[2,3,7,8,12,13,17,18-octabromo-10,15,20-tris(pentafluorophenyl)-21H,23H-porphin-5-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



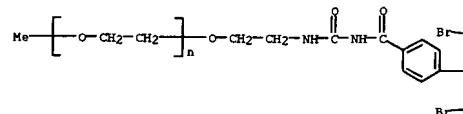
PAGE 2-A



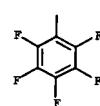
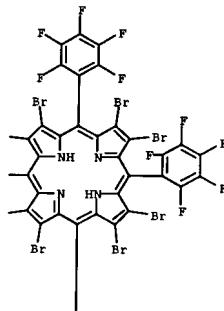
IT 172663-31-9B

RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(photoinduced energy- and electron-transfer of polyethylene glycol-linked fluorinated porphyrin derivs. in lipid bilayers)  
RN 172663-31-9 CAPLUS  
CN Poly(oxy-1,2-ethanediyl),  $\alpha$ -methyl- $\omega$ -(2-[[[4-(2,3,7,8,12,13,17,18-octabromo-10,15,20-tris(pentafluorophenyl)-21H,23H-porphin-5-yl)benzoyl]amino]carbonyl]ethoxy)- (9CI) (CA INDEX NAME)

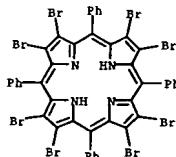
PAGE 1-A



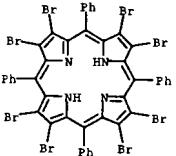
PAGE 1-B



L6 ANSWER 110 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1995:801155 CAPLUS  
DOCUMENT NUMBER: 123:305038  
TITLE: Synthesis and spectroscopic studies of lanthanide monoporphyrinates with meso-tetra-aryl porphyrinate bearing bromines on the  $\beta$ -pyrrole positions and fluorines on phenyl groups  
AUTHOR(S): Spyroulias, G. A.; Coutsopoulos, A. G.  
CORPORATE SOURCE: Chemistry Dep., Univ. Crete, Crete, 71409, Greece  
SOURCE: Polyhedron (1995), 14 (17/18), 2483-90  
CODEN: PLYHDE ISSN: 0277-5387  
PUBLISHER: Elsevier  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The metal derivs. of octabromotetraphenylporphyrin (H2obp) with lanthanide (Sm to Lu) ions were synthesized via the acetylacetonates and characterized by UV-visible, IR and ESR spectroscopies. These lanthanide complexes exhibit interesting electronic features compared with all the previously reported lanthanide monoporphyrinates. The stability of the complexes is discussed in terms of the already known related complexes. The meso-pentafluorophenyl-substituted porphyrin with SmIII was synthesized and its spectroscopic behavior compared with the above B-pyrrole octabromotetraphenyl complexes. IR studies indicate that the axial ligand is the acetylacetonate as was observed for lanthanide monoporphyrinates synthesized by the acetylacetone method. ESR spectroscopy of Ln(obp)acac exhibits one intense peak with  $g$  apprx. 2.00 and hyperfine splitting for Ln = Sm, Eu, Tb, Dy, Ho, Er, Tm, Yb, Lu. The ESR spectrum of Gd(obp)acac exhibits an isotropic  $g$ -factor with a value of 2.3099 and it compared with the analogous complex of Gd(tpp)acac.  
IT 131214-86-39, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(for preparation of rare earth meso-tetraphenyl-octabromoporphyrinato complexes)  
RN 131214-86-3 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



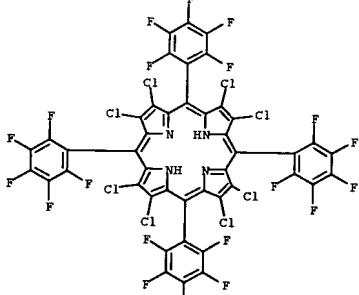
L6 ANSWER 111 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1995:718516 CAPLUS  
 DOCUMENT NUMBER: 123:111720  
 TITLE: Fast atom bombardment mass spectral observations on  $\beta$ -pyrrole-substituted tetraphenylporphyrins  
 AUTHOR(S): Boschi, Tristano; D'Arcangelo, Giuseppe; Tagliatesta, Pietro  
 CORPORATE SOURCE: Dep. di Scienze e Technologie Chimiche, Univ. degli Studi di Roma Tor Vergata, Rome, 00133, Italy  
 SOURCE: Journal of Chemical Research, Synopses (1995), (8), 326-7  
 CODEN: JRPSCD; ISSN: 0308-2342  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The FAB mass spectra of brominated porphyrins have been measured using different matrixes and the fragmentation patterns related to the acidity of the media.  
 IT 131214-86-3  
 RL: PRP (Properties)  
 (fast atom bombardment mass spectral observations on  $\beta$ -pyrrole-substituted tetraphenylporphyrins)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-(9CI) (CA INDEX NAME)



L6 ANSWER 112 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1995:716604 CAPLUS  
 DOCUMENT NUMBER: 123:338859  
 TITLE: Halogenated metalloporphyrin complexes as catalysts for selective reactions of acyclic alkanes with molecular oxygen  
 AUTHOR(S): Lyons, James E.; Ellis, Paul E., Jr.; Myers, Harry K., Jr.  
 CORPORATE SOURCE: Research and Developmental Department, Sun Company, Inc., Marcus Hook, PA, 19061-0835, USA  
 SOURCE: Journal of Catalysis (1995), 155(1), 59-73  
 CODEN: JCTLA5; ISSN: 0021-9517  
 PUBLISHER: Academic  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 123:338859  
 AB We have shown that halogenation of the porphyrin ring of a metalloporphyrin complex can convert a catalytically inactive material into an exceptionally active catalyst for the selective reaction of an alkane with mol. oxygen. The greater the degree of halogenation of the ring, the greater is the catalytic activity of the metal complex. The product profile, while characteristic of radical reactions, is sensitive to the nature of the metal center. Iron complexes are generally more active than those of cobalt, manganese, or chromium. The activity of iron complexes is directly related to the Fe(III)/(II) reduction potential of the porphyrin complex. There is also a similar correlation between the Fe(III)/Fe(II) reduction potential and the rate at which iron haloporphyrin complexes decompose alkyl hydroperoxides. These iron perhaloporphyrin complexes are not only the most active known liquid phase alkane air-oxidation catalysts, they are also the most active hydroperoxide decomposition catalysts known to date. The nature of the products formed is dependent on the structure of the aliphatic substrate that is oxidized and can be rationalized by a catalytic pathway that very efficiently generates alkyl and alkoxy radicals at low temps. The relationship between the electrochemical properties of these complexes and the rates of alkane oxidation and hydroperoxide decomposition lends insight into possible mechanisms of catalytic activity.  
 IT 161405-60-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (halogenated metalloporphyrin complexes as catalysts for alkane oxidation or alkyl hydroperoxide decomposition)  
 RN 161405-60-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 112 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

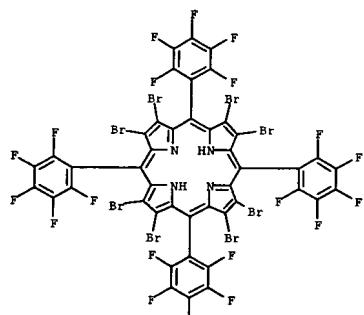
PAGE 1-A



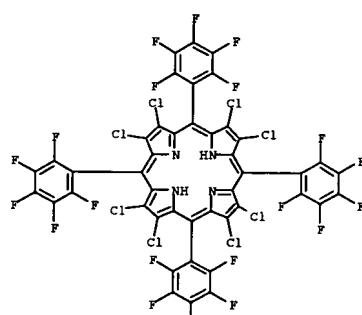
PAGE 2-A

L6 ANSWER 113 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1995:629765 CAPLUS  
 DOCUMENT NUMBER: 123:186498  
 TITLE:  $^{19}F$  NMR Spectra and Structures of Halogenated Porphyrins  
 AUTHOR(S): Birnbaum, Eva R.; Hodge, Julia A.; Grinstaff, Mark W.; Schaefer, William P.; Heeling, Lawrence; Labinger, Jay A.; Bercaw, John E.; Gray, Harry B.  
 CORPORATE SOURCE: Arthur Amos Noyes Laboratory, California Institute of Technology, Pasadena, CA, 91125, USA  
 SOURCE: Inorganic Chemistry (1995), 34(14), 3625-32  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Fluorine-19 NMR spectra of a series of halogenated porphyrins have been used to create a spectral library of different types of fluorine splitting patterns for tetrakis(pentafluorophenyl) porphyrins (TFPP) complexed with diamagnetic and paramagnetic metal ions. The paramagnetic shift, line broadening, and fine structure of the resonances from the peripheral pentafluorophenyl rings are dependent on the symmetry and core environment of the porphyrin macrocycles. In combination with crystal structure data,  $^{19}F$  NMR helps define the behavior of halogenated porphyrins in solution. Six new crystal structures for TFPP and octahalo-TFPP derivs. are reported: H2TFPP in rhombohedral space group R.hivin.3, a = 20.327(4) Å, c = 24.368(5) Å, V = 8720(3) Å<sup>3</sup>, Z = 9; 2nTFPP in monoclinic space group P21/c, a = 12.653(4) Å, b = 11.883(5) Å, c = 15.261(2) Å,  $\beta$  = 103.87(2)°, V = 2227.6(13) Å<sup>3</sup>, Z = 9; CuTFPP in rhombohedral space group R.hivin.3, a = 20.358(5), c = 24.347(6) Å, V = 8739(4) Å<sup>3</sup>, Z = 9; H2TFPPCl8 in triclinic space group P.hivin.1, a = 11.066(1) Å, b = 14.641(3) Å, c = 14.678(2) Å,  $\alpha$  = 88.97(1),  $\beta$  = 76.05(1)°,  $\gamma$  = 71.29(1)°, V = 2181.4(6) Å<sup>3</sup>, Z = 2; 2nTFPPCl8 in tetragonal space group P.hivin.421c, a = 19.502(20), c = 19.916(8) Å, V = 4152(6) Å<sup>3</sup>; H2TFPPBr8 in monoclinic space group C2, a = 27.634(6) Å, b = 6.926(2) Å, c = 14.844(3) Å,  $\beta$  = 109.64(2)°, V = 2675.8(11) Å<sup>3</sup>, Z = 2.  
 IT 139944-26-6P 161405-60-3P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 ( $^{19}F$  NMR spectra and structures of halogenated porphyrins)  
 RN 139944-26-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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RN 161405-60-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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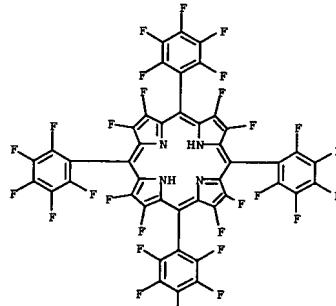
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L6 ANSWER 114 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 ACCESSION NUMBER: 1995:508382 CAPLUS  
 DOCUMENT NUMBER: 1221290548  
 TITLE: Substituent Effects on Valence Ionization Potentials of Free Base Porphyrins: A Local Density Functional Study  
 AUTHOR(S): Ghosh, Abhik  
 CORPORATE SOURCE: Department of Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA  
 SOURCE: Journal of the American Chemical Society (1995), 117(16), 4691-9  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: CODEN: JACSAI; ISSN: 0002-7863  
 LANGUAGE: English  
 AB Local d. functional (LDF) calcns. with polarized double- $\zeta$  basis sets have been used to calculate the two lowest one-electron ionization potentials of a variety of free base porphyrins with multiple alkyl, aryl, fluoro, chloro, bromo, trifluoromethyl, cyano, and nitro substituents. For unsubstituted porphyrin (PH2),  $\beta$ -octaalkylporphyrins, and meso-tetracyanoporphyrin (TPPH2), LDF-ASCF calcns. reproduce the lowest UV photoelectron spectral (UPS) IPs to within  $\approx$ 0.2 eV. The two lowest one-electron IPs of TPPH2 are predicted to be lower than those of PH2 by  $\approx$ 0.5 eV, in agreement with UPS expts. Ab initio Hartree-Fock (HF) theory seriously underestimates this electronic effect of meso-tetra-Ph substitution. Both LDF and HF theories predict that substituents on the Ph rings of TPPH2 should strongly affect the lowest one-electron IPs of TPPH2. Substitution of the para positions of the Ph groups of TPPH2 with  $-\text{CF}_3$ ,  $-\text{CN}$ , or  $-\text{NO}_2$  substituents should raise the lowest IP by 0.7-0.8 eV, while fluorination of the Ph rings should increase the lowest IP by  $\approx$ 0.95 eV. A comparison of the IPs of ortho-, meta-, and para-fluorinated TPPH2 derivs. suggests that electron-withdrawing substituents at meta and para positions should exert significantly stronger electronic effects on the porphyrin ring than ortho substituents. Ab initio HF theory seriously overestimates the electron-withdrawing effect of peripheral halogen substituents. Provided there is no macrocycle buckling due to steric interactions among peripheral substituents, LDF theory predicts that meso-tetrahalogenation (with F, Cl, or Br) should have almost no influence on the lowest IP of PH2, while  $\beta$ -octachlorination or octabromination should increase the lowest IP by  $\approx$ 0.4-0.5 eV. Electrochemical measurements support these LDF predictions.  $\beta$ -Octafluorination is predicted to exert an electronic effect of  $\approx$ 0.85 eV on the lowest IPs of PH2, which is significantly larger than the electronic effect of  $\beta$ -octachlorination or octabromination. Substituents such as  $-\text{CF}_3$ ,  $-\text{CN}$ , and  $-\text{NO}_2$  exert far higher electronic effects than the halogens. For instance, LDF theory predicts that the lowest IP of meso-tetraakis(trifluoromethyl)porphyrin should exceed that of TPPH2 by  $\approx$ 1.74 eV and that of meso-tetrakis(pentafluorophenyl)porphyrin by  $\approx$ 0.68 eV. Unlike the halogens, meso-tetrabromination with cyano groups should drastically increase the lowest IP of PH2, by a margin of  $\approx$ 1.2 eV.  $\beta$ -Octacyano-substitution is predicted to have an electronic effect of  $>2.0$  eV on the lowest IP of PH2. Meso-tetranitrosubstitution is predicted to elevate the lowest IP of PH2 by  $\approx$ 0.9-1.1 eV, depending on the conformation of the nitro groups. In general, meso-substituents exert stronger electronic effects than the same substituents placed at  $\beta$ -positions.

IT 121399-88-0 144811-81-4, Octachloroporphine  
 144811-83-6, Octabromoporphine 144811-86-9,  
 Octafluoroporphine

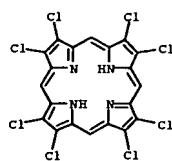
L6 ANSWER 114 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 RL: FRP (Properties)  
 (local d. function study of substituent effects on valence ionization potentials of porphyrins)  
 RN 121399-88-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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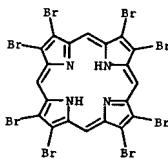
PAGE 2-A

RN 144811-81-4 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

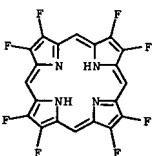


RN 144811-83-6 CAPLUS

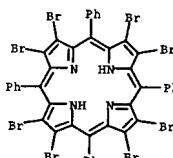
L6 ANSWER 114 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



RN 144811-86-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)



L6 ANSWER 115 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1995:476115 CAPLUS  
 DOCUMENT NUMBER: 122:290549  
 TITLE: Synthesis of beta-aryl substituted porphyrins by palladium catalyzed Suzuki cross-coupling reactions  
 AUTHOR(S): Chan, Kin Shing; Zhou, Xiang; Au, Ming Tak; Tam, Chak Yue  
 CORPORATE SOURCE: Department of Chemistry, The Chinese Univ. of Hong Kong, Shatin, Hong Kong  
 SOURCE: Tetrahedron (1995), 51(11), 3129-36  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 122:290549  
 AB  $\beta$ -Bromoporphyrins undergo Suzuki cross coupling reactions with aryl boronic acids  $p$ -X-C<sub>6</sub>H<sub>4</sub>B(OH)<sub>2</sub> (X = H, Me, MeO, Cl) to give  $\beta$ -arylporphyrins in high yields.  
 IT 131214-86-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of  $\beta$ -arylporphyrins by palladium-catalyzed Suzuki cross-coupling with arylboronic acids)  
 RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

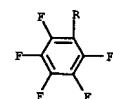


L6 ANSWER 116 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1995:465601 CAPLUS  
 DOCUMENT NUMBER: 122:23871  
 TITLE: Metal complexes of substituted gable porphyrins as oxidation catalysts.  
 INVENTOR(S): Lyons, James E.; Ellis, Paul E., Jr.; Wagner, Richard W.  
 PATENT ASSIGNEE(S): Sun Co., Inc., USA  
 SOURCE: Eur. Pat. Appl., 6 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

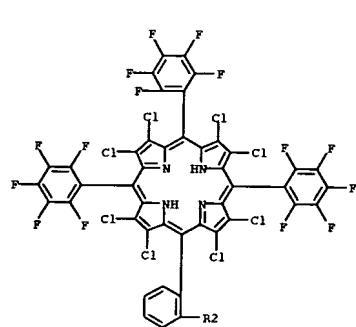
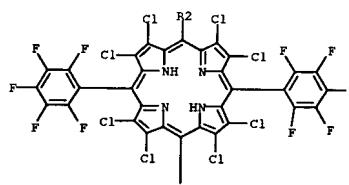
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 636628	A1	19950201	EP 1994-305634	19940729
R: BE, DE, FR, GB, IT, NL				
US 5480986	A	19960102	US 1993-100516	19930730
CA 2129055	AA	19950131	CA 1994-2129055	19940728
JP 07089964	AA	19950404	JP 1994-197953	19940729
PRIORITY APPLN. INFO.:			US 1993-100516	A 19930730
OTHER SOURCE(S): MARPAT 122:223071				
AB	Transition metal complexes of Gable porphyrins having two porphyrin rings connected through a linking group, and having on the porphyrin rings electron-withdrawing groups, such as halogen, nitro or cyano, are useful as catalysts for the oxidation of organic compds., e.g. alkanes.			
IT 162023-49-62				
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)				
(metal complexes of substituted Gable porphyrins as oxidation catalysts)				
RN 162023-49-6 CAPLUS				
CN 21H,23H-Porphine, 5,5'-(1,2-phenylene)bis[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(pentafluorophenyl)- (9CI) (CA INDEX NAME)				

L6 ANSWER 116 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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L6 ANSWER 117 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1995:448372 CAPLUS  
 DOCUMENT NUMBER: 122:203772  
 TITLE: Electronic Structures of Halogenated Ruthenium Porphyrins. Crystal Structure of RuTPPC18(CO)H<sub>2</sub>O (TPPC18 = Octa- $\beta$ -chlorotetrakis(pentafluorophenyl)porphyrin)  
 AUTHOR(S): Birnbaum, Eva R.; Schaefer, William P.; Labinger, Jay A.; Bercaw, John E.; Gray, Harry B.  
 CORPORATE SOURCE: Arthur Amos Noyes Laboratory, California Institute of Technology, Pasadena, CA, 91125, USA  
 SOURCE: Inorganic Chemistry (1995), 34(7), 1751-5  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Ru(II) octa- $\beta$ -halotetrakis(pentafluorophenyl)porphyrins (RuTPPCX<sub>2</sub>(CO), RuTPPC18(py)2; X = Cl, Br) were synthesized, and the crystal structure of RuTPPC18(CO)H<sub>2</sub>O was determined: monoclinic, space group P21/c, a 14.364(3), b 16.012(4), c 26.679(8) Å,  $\beta$  90.29(2) $^\circ$ , Z = 4,  $R_w$  = 0.028 on F2 for 8005 reflections,  $R$  = 0.067 for 5378 reflections with  $F_0 > 3\sigma(F_0)$ ; the porphyrin is highly distorted, with a 1.19 Å maximum displacement of the  $\beta$ -Cl atoms from the mean porphyrin plane. The reduction potentials of RuTPPCX<sub>2</sub> complexes are

P21/c, a 14.364(3), b 16.012(4), c 26.679(8) Å,  $\beta$  90.29(2) $^\circ$ , Z = 4,  $R_w$  = 0.028 on F2 for 8005 reflections,  $R$  = 0.067 for 5378 reflections with  $F_0 > 3\sigma(F_0)$ ; the porphyrin is highly distorted, with a 1.19 Å maximum displacement of the  $\beta$ -Cl atoms from the mean porphyrin plane. The reduction potentials of RuTPPCX<sub>2</sub> complexes are

much more pos. (> 0.5 V) than those of unhalogenated analogs, owing to the influence of the electron-withdrawing X atoms. The relatively high energies of the Soret bands in the RuTPPCX<sub>2</sub> electronic spectra are consistent with an electronic structural model involving RuII back-bonding to the porphyrin  $ex^*$  orbitals.

IT 139944-26-6, Octa- $\beta$ -bromotetrakis(pentafluorophenyl)porphyrin  
 161405-60-3, Octa- $\beta$ -chlorotetrakis(pentafluorophenyl)porphyrin

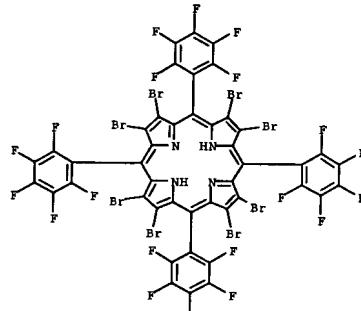
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (for preparation of ruthenium halogenated porphyrinato complexes)

RN 139944-26-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 117 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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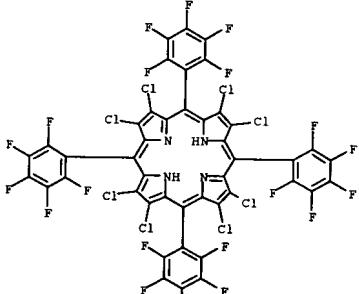
PAGE 2-A

RN 161405-60-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 117 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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L6 ANSWER 118 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

1995:280591 CAPLUS

ACCESSION NUMBER: 122:187199

TITLE: Sterically strained porphyrins - effect of nuclear protonation and peripheral substituents on the conformation in tetra-meso-, octa- $\beta$ -, and dodeca-substituted porphyrin dications

AUTHOR(S): Senge, Mathias O.; Forsyth, Timothy P.; Nguyen, Liem T.; Smith, Kevin M.  
 CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616, USA  
 SOURCE: Angew. Chem., Int. Ed. Engl., 1994, 33(23/24), 2554-7 (See also Angew. Chem., Int. Ed. Engl., 1994, 33(23/24), 2485-7)

PUBLISHER: VCH

DOCUMENT TYPE: Journal

LANGUAGE: German

AB The conformations of meso-tetra-,  $\beta$ -octa-, and dodeca-substituted porphyrin dications are discussed.

IT 161614-78-4

RL: PRP (Properties)  
 (effect of nuclear protonation and peripheral substituents on the conformation in tetra-meso-, octa- $\beta$ -, and dodeca-substituted porphyrin dications)

RN 161614-78-4 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,13,20-tetraphenyl-, bis(trifluoroacetate), compd. with trichloromethane (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 67-66-3

CMF C H Cl



CM 2

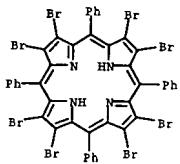
CRN 161614-77-3

CMF C44 H22 Br8 N4 . 2 C2 H F3 O2

CM 3

CRN 131214-86-3

CMF C44 H22 Br8 N4



CH 4

CRN 76-05-1  
CMF C2 H F3 O2

TITLE: Ab Initio Hartree-Fock and Local Density Functional Calculations on Prototype Halogenated Porphyrins. Do Electrochemically Measured Substituent Effects Reflect Gas-Phase Trends?

AUTHOR(S): Ghosh, Abhik

CORPORATE SOURCE: Department of Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA

SOURCE: Journal of Physical Chemistry (1994), 98(43), 11004-6

CODEN: JPCHAZ ISSN: 0022-3654

DOCUMENT TYPE: Journal

LANGUAGE: English

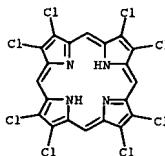
AB First-principles quantum chemical methods have been employed to simulate and predict the electronic effects of peripheral polyhalogenation in porphyrins. Spin-RHF theory performs unexpectedly poorly in calcns. of valence ionization potential of polyhalogenated porphyrins. In contrast, the results of local d. functional calcns. of the lowest ionization potentials of free base porphyrin, meso-tetrafluoroporphyrin, and  $\beta$ -octachloroporphyrin are consistent with existing electrochem. information.IT 144811-81-4,  $\beta$ -Octachloroporphyrin

RL: PRP (Properties)

(ab initio Hartree-Fock and local d. functional calcns. of substituent effects in halogenated porphyrins)

RN 144811-81-4 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)

TITLE: Synthesis of  $\beta$ -octasubstituted sterically bulky porphyrins by Suzuki cross coupling

AUTHOR(S): Zhou, Xiang; Zhou, Zhong-yuan; Mak, Thomas C. W., Chan, Kin Shin

CORPORATE SOURCE: Dep. Chem., Chin. Univ. Hong Kong, Shatin, Hong Kong  
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1994), (18), 2519-20

CODEN: JCPRB4 ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:300639

AB  $\beta$ -Octasubstituted tetramesitylporphyrins have been prepared in good yields by Suzuki cross coupling of  $\beta$ -octabromotetramesitylporphyrin with aryl- and alkyl-boronic acids. A single-crystal X-ray anal. of  $\beta$ -octamethyltetramesitylporphyrin shows a saddled non-planar structure.

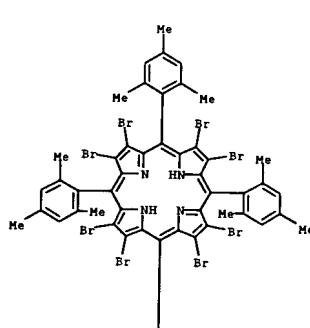
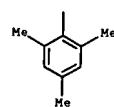
IT 129006-48-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(Suzuki cross coupling with boronic acids)

RN 129006-48-0 CAPLUS

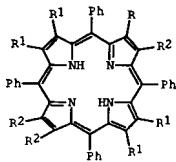
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1994435121 CAPLUS

DOCUMENT NUMBER: 121:35121

**TITLE:** Synthesis of  $\beta$ -aryl substituted porphyrins by palladium-catalyzed cross-coupling reactions  
**AUTHOR(S):** Chan, Xia-Shing; Zhou, Xiang; Luo, Bao-Sheng; Mak, Thomas C. W.  
**CORPORATE SOURCE:** Dep. Chem., Chin. Univ. Hong Kong, Shatin, Hong Kong  
**SOURCE:** Journal of the Chemical Society, Chemical Communications (1994), (3), 271-2  
**CODEN:** JCCCAT; ISSN: 0022-4936  
**DOCUMENT TYPE:** Journal  
**LANGUAGE:** English  
**GI**



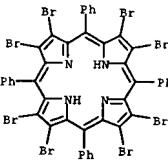
**AB**  $\beta$ -Bromoporphyrins I ( $R = Br$ ,  $R1 = R2 = H$ ;  $R = R2 = Br$ ;  $R = R1 = R2 = Br = Br$ ) undergo Suzuki cross-coupling reactions with aryl boronic acids to give  $\beta$ -arylporphyrins I ( $R = Ar$ ,  $R1 = R2 = H$ ;  $R = R2 = H$ ,  $R1 = Ar$ ;  $R = R1 = R2 = Ar$ ;  $Ar = Ph$ , 4-MeC6H4, 4-MeOC6H4, 4-Me3C6H4, 4-ClC6H4) in high yields and x-ray anal. shows that H2TPP(Ph)4 I ( $R = R2 = H$ ,  $R1 = Ph$ ) (TPP = tetraphenylporphyrin) is centrosym. and possesses a hydrogen-bonded inner core.

IT 131214-86-3

RL: PRP (Properties)  
(palladium-catalyzed cross-coupling of, with aryl boronic acids)

RN 131214-86-3 CAPLUS

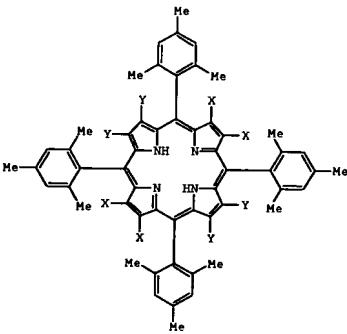
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1994435117 CAPLUS

DOCUMENT NUMBER: 121:35117

**TITLE:** Effect of conformation on the redox potentials of porphyrins halogenated in the  $\beta$ -pyrrole positions  
**AUTHOR(S):** Ochsenbein, Philippe; Ayogou, Khadija; Mandon, Dominique; Fischer, Jean; Weiss, Raymond; Austin, Rachel N.; Jayaram, Karupiah; Gold, Avram; Terner, James; Fajer, Jack  
**CORPORATE SOURCE:** Inst. Le Bel, Univ. Louis Pasteur, Strasbourg, F-67070, Fr.  
**SOURCE:** Angewandte Chemie (1994), 106(3), 355-7 (See also Angew. Chem., Int. Ed. Engl., 1994, 106(3), 348-50)  
**CODEN:** ANCEAD; ISSN: 0044-8249  
**DOCUMENT TYPE:** Journal  
**LANGUAGE:** German  
**GI**



**AB** The porphyrins I [ $X = Y = H$ ,  $Cl$ ,  $Br$ ;  $X = Cl$ ,  $Br$ ,  $Y = H$ ] were prepared and their redox potentials and crystal structures were compared. Increasing halogenation in I is accompanied by increasing twist in the mol. I [ $X = Cl$ ,  $Br$ ,  $Y = H$ ] were more difficult to reduce than I [ $X = Y = H$ ], but I [ $X = Y = Cl$ ,  $Br$ ] were more easily oxidized than I [ $X = Cl$ ,  $Br$ ,  $Y = H$ ].

IT 155586-24-6

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

RN 155586-24-6 CAPLUS

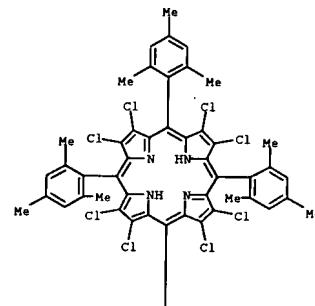
CN Methanol compd. with 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-21H,23H-porphine (2:1) (SCI) (CA INDEX NAME)

CH 1

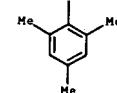
CRN 152037-87-1

CMF C56 H46 Cl8 N4

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CH 2

CRN 67-56-1

CMF C H4 O

H3C-OH

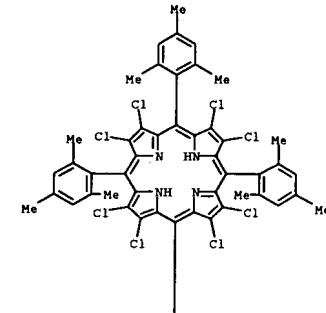
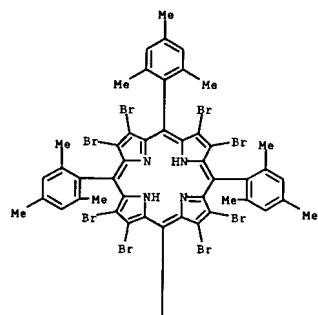
IT 129006-48-0P 152037-87-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, redox potential, and conformation of)

RN 129006-48-0 CAPLUS

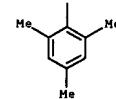
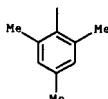
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-

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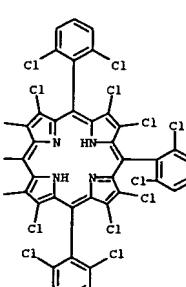
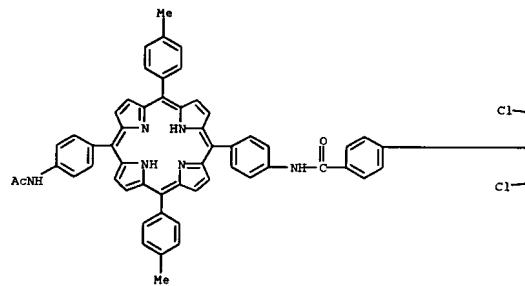
PAGE 2-A

RN 152037-87-1 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 123 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1994-311114 CAPLUS  
DOCUMENT NUMBER: 120-311114  
TITLE: Free Energy Dependence of Photoinduced Charge Separation Rates in Porphyrin Dyads  
AUTHOR(S): Degraiano, Janice M.; Liddell, Paul A.; Leggett, Loral Moore, Ana L.; Moore, Thomas A.; Gust, Devens  
CORPORATE SOURCE: Center for the Study of Early Events in Photosynthesis, Arizona State University, Tempe, AZ, 85287, USA  
SOURCE: Journal of Physical Chemistry (1994), 98(7), 1758-61  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A series of covalently linked porphyrin dyads in which the thermodynamic driving force for interporphyrin photoinduced charge separation spans a range of 1.13 eV has been prepared. Time-resolved fluorescence studies have yielded 22 rate constants for photoinduced electron transfer in dichloromethane solution ranging from 4.1 + 107 to 5.0 + 1011 s-1. The data are consistent with the theoretical treatments of R. Marcus (1956) and V. Levich (1966), although there is no evidence for inverted behavior. In the normal region, electron transfer between free base porphyrin molecules is about 10 times faster than transfer involving a zinc porphyrin and having the same thermodynamic driving force, based on electrochemical measurements. Photoinduced electron transfer to an excited singlet state and electron transfer from an excited singlet state have the same dependence upon free energy change.  
IT 154891-85-7 154891-86-8 154891-87-9  
154986-34-2 154986-35-3 155208-76-7  
RL: PRP (Properties)  
(photoinduced intramol. electron transfer in, free energy dependence of)  
RN 154891-85-7 CAPLUS  
CN Benzamide, N-[4-(4-(acetylaminophenyl)-10,20-bis(4-methylphenyl)-21H,23H-porphin-5-yl)phenyl]-4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(2,6-dichlorophenyl)-21H,23H-porphin-5-yl]- (9CI) (CA INDEX NAME)

L6 ANSWER 123 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

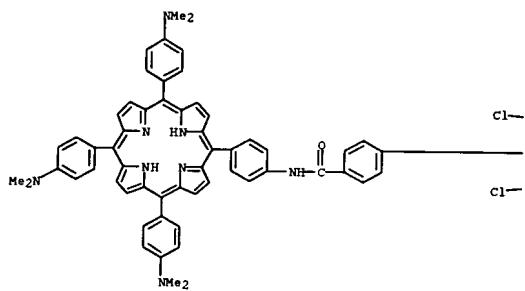
PAGE 1-A



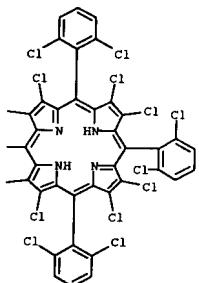
PAGE 1-B

RN 154891-86-8 CAPLUS  
CN Benzamide, 4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(2,6-dichlorophenyl)-21H,23H-porphin-5-yl]-N-(4-[10,15,20-tris(4-(dimethylaminophenyl)-21H,23H-porphin-5-yl)phenyl]- (9CI) (CA INDEX NAME)

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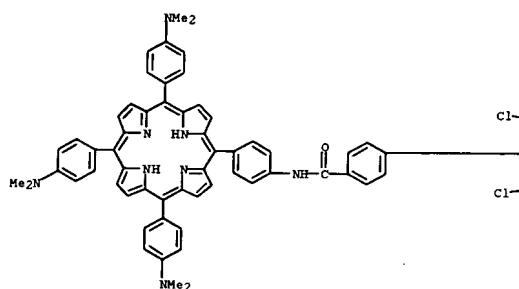


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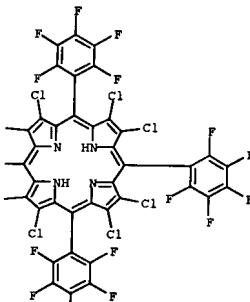


RN 154891-87-9 CAPLUS  
 CN Benzamide, 4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(pentafluorophenyl)-21H,23H-porphin-5-yl]-N-[4-(10,15,20-tris[4-(dimethylamino)phenyl]-21H,23H-porphin-5-yl)phenyl]- (9CI) (CA INDEX NAME)

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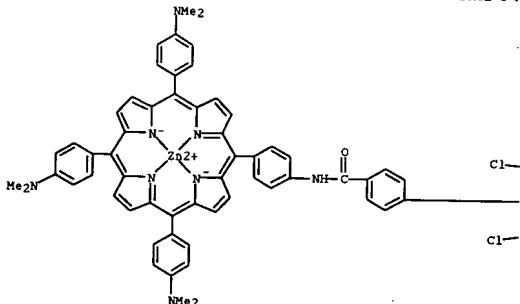


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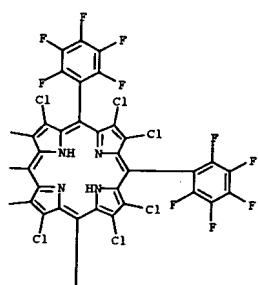


RN 154986-34-2 CAPLUS  
 CN Zinc, [4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(pentafluorophenyl)-21H,23H-porphin-5-yl]-N-[4-(10,15,20-tris[4-(dimethylamino)phenyl]-21H,23H-porphin-5-yl)phenyl]benzamidato(2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

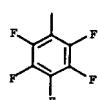
PAGE 1-A



PAGE 1-B

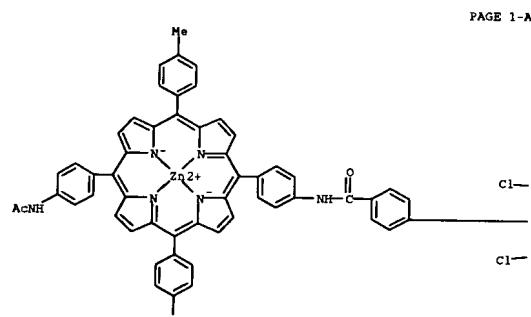


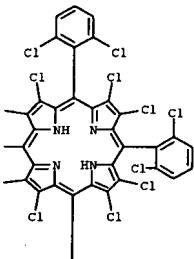
PAGE 2-B



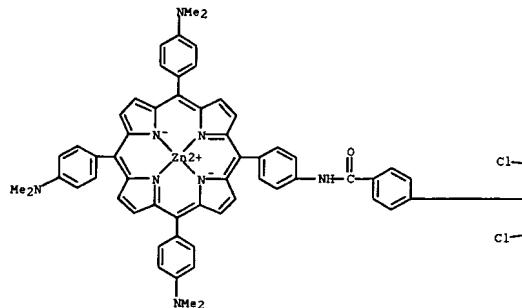
RN 154986-35-3 CAPLUS  
 CN Zinc, [N-[4-(15-(4-acetylaminophenyl)-10,20-bis(4-methylphenyl)-21H,23H-porphin-5-yl)phenyl]-4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(2,6-dichlorophenyl)-21H,23H-porphin-5-yl]benzamidato(2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

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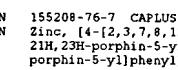




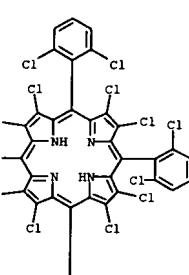
PAGE 1-B



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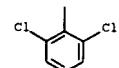


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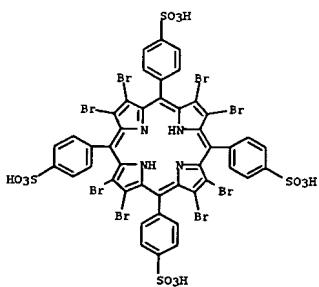
RN 155208-76-7 CAPLUS  
 CN Zinc, [4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(2,6-dichlorophenyl)-21H,23H-porphin-5-yl]-N-[4-[10,15,20-tris(4-(dimethylamino)phenyl)-21H,23H-porphin-5-yl]phenyl]benzamidato(2-)-, (SP-4-2)- (9CI) (CA INDEX NAME)

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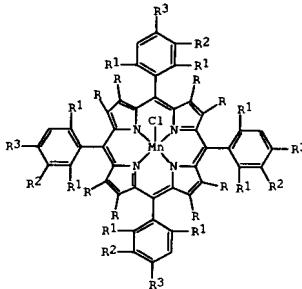
PAGE 2-B

L6 ANSWER 124 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1994:283247 CAPLUS  
 DOCUMENT NUMBER: 120:283247  
 TITLE: Resonance light-scattering studies of porphyrin diacid aggregates  
 AUTHOR(S): Pasternack, Robert F.; Schaefer, Kurt F.; Hambricht, Peter  
 CORPORATE SOURCE: Department of Chemistry, Swarthmore College, Swarthmore, PA, 19081, USA  
 SOURCE: Inorganic Chemistry (1994), 33(9), 2062-5  
 CODEN: INOCAJ; ISSN: 0020-1669  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Resonance light scattering measurements were used to investigate the solute species present in acidic aqueous media for some 14 sulfonated porphyrins. The anomalous absorption band in the Soret region reported for several of these porphyrins arises from the formation of extended aggregates of electronically coupled chromophores and illustrate the sensitivity and specificity of this unconventional light scattering method.  
 IT 154783-99-0  
 RL: PRP (Properties)  
 (resonance light scattering visible spectra of aggregates of)  
 RN 154783-99-0 CAPLUS  
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphin-5,10,15,20-tetrayl)tetraakis- (9CI) (CA INDEX NAME)



L6 ANSWER 125 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1994:134113 CAPLUS  
 DOCUMENT NUMBER: 120:134113

TITLE: Catalytic activity and chemical stability of perhalogenated manganese(II)-tetraarylporphyrins in alkene epoxidations  
 AUTHOR(S): Banfi, Stefano; Mandelli, Roberta; Montanari, Fernando; Quici, Silvio  
 CORPORATE SOURCE: Dip. Chim. Org. Ind., Univ. Milano, Milano, I-20133, Italy  
 SOURCE: Gazzetta Chimica Italiana (1993), 123(7), 409-15  
 DOCUMENT TYPE: CODEN: GCITA9; ISSN: 0016-5603  
 LANGUAGE: English  
 GI



I

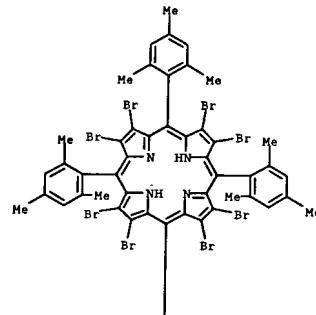
AB Structural factors, which govern the chemical stability of metallotetraarylporphyrins I ( $R = H, Cl$ ,  $R_1 = Cl$ ,  $R_2 = H, NO_2$ ,  $R_3 = H$ ;  $R = H, Br$ ,  $R_1 = R_3 = Me$ ,  $R_2 = H, R = Me$ ,  $R_1 = Cl$ ,  $R_2 = R_3 = H$ ) were investigated in  $CH_2Cl_2/H_2O$  two-phase alkene epoxidations, promoted by aqueous  $NaCl$  or  $30\% H_2O_2$ . In contrast to recent literature reports, the perhalogenation of pyrrole  $\beta$ -positions of tetraarylporphyrins decreases the reactivity and the robustness of these catalysts with respect to the unsubstituted ones. The only exception is provided by I ( $R = Br$ ,  $R_1 = R_3 = Me$ ,  $R_2 = H$ ,  $R = H$ ), which proved to be more efficient than I ( $R = H$ ,  $R_1 = R_3 = Me$ ,  $R_2 = H$ ). Nevertheless II is far less reactive than I ( $R = R_2 = R_3 = H$ ,  $R_1 = Cl$ ). The influence of external factors, such as Mn-porphyrin/oxidant/substrate ratios and that of the axial ligand, was also examined. It was demonstrated that the assessed stability of perhalogenated tetraarylporphyrins is subject to operative conditions where a large excess of substrate is used with respect to the oxidant, conditions which are difficult to use on a preparative scale.

IT 129006-48-0P 134833-67-3P

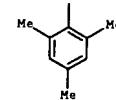
RL: SPN (Synthetic preparation); PREP (Preparation)

L6 ANSWER 125 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 (intermediate in prep. of perhalogenated manganese(II)-tetraarylporphyrins)  
 RN 129006-48-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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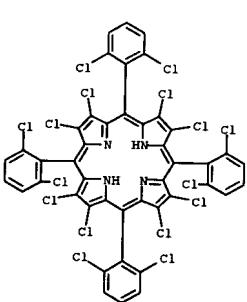


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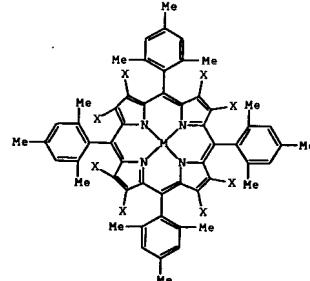


RN 134833-67-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 125 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L6 ANSWER 125 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1994:67865 CAPLUS  
 DOCUMENT NUMBER: 120:67865  
 TITLE: The oxoiron  $\kappa$  cation radical of meso-tetramesitylporphyrin chlorinated in the eight  $\beta$  positions: electronic and structural properties  
 AUTHOR(S): Ochseneck, Philippe; Mandon, Dominique; Fischer, Jean; Weiss, Raymond; Austin, Rachel; Jayaraj, Karupiah; Gold, Avram; Turner, James; Bill, Eckhardt, et al.  
 CORPORATE SOURCE: Inst. LeBel, Univ. Louis Pasteur, Strasbourg, F-67070, FR.  
 SOURCE: Angewandte Chemie (1993), 105(10), 1504-5 (See also Angew. Chem. Int. Ed. Engl., 1993, 32(10), 1437-39)  
 DOCUMENT TYPE: CODEN: ANCEAD; ISSN: 0044-8249  
 LANGUAGE: Journal German  
 GI

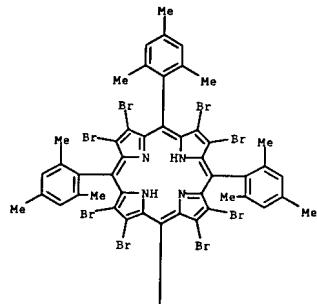


I

AB I ( $M = FeCl$ ,  $X = Cl$ ,  $Br$ ) were prepared by the metalation of I ( $M = H_2$ ) with  $FeCl_2$ .  $I \cdot H_2O$  are tetragonal, space group  $P\bar{h}i\bar{v}i\bar{n}$ ,  $a = 421\text{ \AA}$ ,  $c = 2$ ,  $R/R_w = 0.069/0.091$  and  $0.053/0.075$ , resp. The Fe in I ( $M = FeCl$ ,  $X = Cl$ ,  $Br$ ) lies  $0.55(1)\text{ \AA}$  above the plane of the  $4N$  atoms. The average deviations of the  $\beta$ -C atoms from the plane are  $0.87$  and  $0.90\text{ \AA}$  for I ( $M = FeCl$ ,  $X = Cl$ ,  $Br$ ), resp., in comparison to  $0.90$  and  $0.95\text{ \AA}$  for I ( $M = H_2$ ,  $X = Cl$ ,  $Br$ ), resp. I ( $M = FeCl$ ,  $X = Cl$ ,  $Br$ ) were oxidized by  $m$ -chloroperoxybenzoic acid at  $-80^\circ$  to give in toluene I ( $M = FeO$ ,  $X = Cl$ ,  $Br$ ) which were ESR-inactive but in  $CH_2Cl_2$  ESR-active. I ( $M = FeO$ ,  $X = Cl$ ) was observed. The ESR data for I ( $M = FeO$ ,  $X = Cl$ ) is typical for a quartet ground state of  $S = 3/2$  and indicated that ferromagnetic coupling occurs between the low-spin Fe(IV) center and the porphyrin  $\pi$ -radical cation. The temperature dependence of the exchange coupling is described using the 3-state model of the Kramer-doublet. Comparison of the spectral properties of I ( $M = FeO$ ,  $X = Cl$ ) with those of I ( $M = FeO$ ,  $X = H$ ) indicate that they have similar

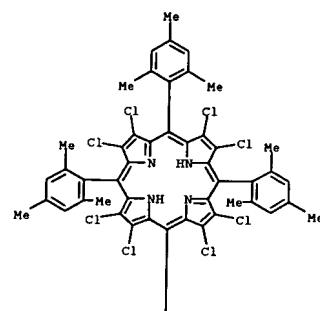
L6 ANSWER 126 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 electronic structures.  
 129006-48-0 152037-87-1  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and mol. structure and oxidation of, by peroxybenzoic acid)  
 RN 129006-48-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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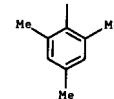


L6 ANSWER 126 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

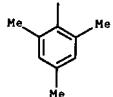
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RN 152037-87-1 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 127 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1993:594357 CAPLUS  
 DOCUMENT NUMBER: 119:194357

TITLE: Electrochemical and spectroelectrochemical behavior of cobalt(III), cobalt(II), and cobalt(I) complexes of meso-tetraphenylporphyrinate bearing bromides on the  $\beta$ -pyrrole positions

AUTHOR(S): D'Souza, Francis; Villard, Anne; Van Caemelbecke, Eric; Franzen, Michelle; Boschi, Tristano; Tagliatesta, Pietro; Kadish, Karl M.

CORPORATE SOURCE: Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA

SOURCE: Inorganic Chemistry (1993), 32(19), 4042-8

CODEN: INOCAU; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

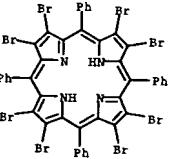
AB The synthesis and characterization of (meso-tetraphenylporphyrinato)cobalt (II) complexes containing 6, 7, or 8 Br groups at the  $\beta$ -pyrrole positions of the macrocycle are reported. Each compound undergoes 3 1-electron oxidations, and up to 9 1-electron redns. depending upon the degree of Br substitution. The 1st reduction yields  $[(TPPBr_8)Co]^{1+}$  while the 1st oxidation gives  $[(TPPBr_8)Co]^{3+}$  where (TPPBr<sub>8</sub>) is the dianion of the brominated tetraphenylporphyrin. Cyclic voltammetry studies reveal a pos. shift of the metal and ring-centered redox potentials of the bromoporphyrins as compared to E<sub>1/2</sub> for the reduction and oxidation of unsubstituted

(TPP)Co. The optical absorption spectra of each electrogenerated Co(II) and Co(III) complex were recorded in a thin-layer cell and show that the transition energies for both the Soret and visible bands vary as a function of Br groups on the porphyrin periphery. The electron withdrawing Br substituents also produce a red shift in the Soret and visible bands of the porphyrin which follows the order:  $(TPPBr_8)Co > (TPPBr_7)Co > (TPPBr_6)Co > (TPP)Co$ . The singly oxidized and singly reduced products are stable on the cyclic voltammetric and thin-layer time scales, but further reduction beyond  $[(TPPBr_8)Co]^{1+}$  lead to the stepwise elimination of Br groups to give  $[(TPP)Co]^{1-}$  as a final product in solution. Results obtained by controlled-potential thin-layer spectroelectrochem. and rotating ring disk electrode voltammetry confirm this expected observation.

IT 131214-86-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with cobalt acetate)

RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



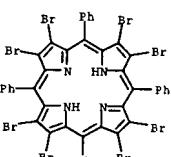
L6 ANSWER 127 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L6 ANSWER 127 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L6 ANSWER 127 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L6 ANSWER 128 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1993:547430 CAPLUS  
 DOCUMENT NUMBER: 119:147430  
 TITLE: Structure of nonplanar octabromotetraphenylporphyrin and kinetics of rapid metalation reactions  
 AUTHOR(S): Bhryappa, Puttaih; Nethaji, Munirathnam; Krishnan, Varadachari  
 CORPORATE SOURCE: Dep. Inorg. Phys. Chem., Indian Inst. Sci., Bangalore, 560 012, India  
 SOURCE: Chemistry Letters (1993), (5), 869-72  
 CODEN: CHLTAG; ISSN: 0366-7022  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The crystal structure of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin (H2L) shows that it adopts a severe saddle-shaped distorted structure owing to the steric crowding of heavy Br substituents. Kinetic studies indicate the rate enhancement of H2L metalation reaction is primarily due to the nonplanarity of the ring while the electronic effect diminishes the affinity of the porphyrin towards metal ions.  
 IT 150045-60-6, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin diethanolate dihydrate  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (crystal structure and kinetics of metalation of, by transition metal(II) cations)  
 RN 150045-60-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with ethanol (1:2), dihydrate (9CI) (CA INDEX NAME)

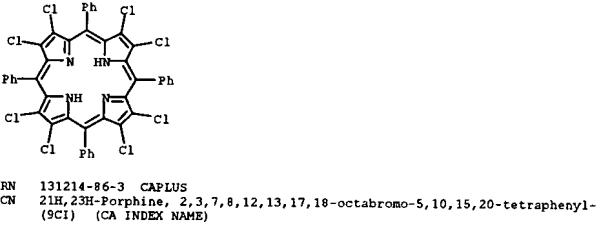
CH 1  
 CRN 131214-86-3  
 CMF C44 H22 Br8 N4



CM 2  
 CRN 64-17-5  
 CMF C2 H6 O

H3C-CH2-OH

L6 ANSWER 129 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1993:191408 CAPLUS  
 DOCUMENT NUMBER: 118:191408  
 TITLE: Structure of meso-tetraaryl- $\beta$ -octahalogenoporphyrins: a semi-empirical quantum-mechanical investigation  
 AUTHOR(S): Brigaud, O.; Battioni, P.; Mansuy, D.  
 CORPORATE SOURCE: Lab. Chim. Biochim. Pharmacol. Toxicol., Univ. Rene Descartes, Paris, 75270, Fr.  
 SOURCE: New Journal of Chemistry (1992), 16(11), 1031-8  
 CODEN: NJCHES; ISSN: 0398-9836  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB AM1 calcns. were performed on 3 series of porphyrins, namely  $\beta$ -octahalogenoporphyrins, meso-tetraphenylporphyrins and on their zinc complexes. In the case of meso-tetraphenylporphyrins and  $\beta$ -octahalogenoporphyrins, a planar structure of the tetrapyrrole ring is the most stable one, as expected. On the contrary, the preferred conformation of meso-tetraphenyl- $\beta$ -octabromo(chloro)porphyrine and their zinc complexes corresponds to a saddle shape structure. For instance, the saddle conformation of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin is more stable by 59 kJ/mol than the corresponding planar conformation. The best, energy wise, conformations are obtained by rotation of the pyrrole rings about the Cmeso-Cmeso lines and only to a much smaller extent about the pyrrole Ca-Ca lines. The stability of the conformations in which the meso carbons are no longer in the same plane (twist) decreases rapidly with the magnitude of this distortion. For saddle shape conformations, the Ph rings are no longer perpendicular to the porphyrin mean plane. The presence of bulky substituents on both  $\beta$  and meso carbon atoms is essential to obtain this type of structure. These results are in good agreement with recent x-ray studies on  $\beta$ -substituted meso-tetraarylporphyrins. The variation of the spacing and ordering of the frontier orbitals obtained in ruffled porphyrins is discussed in relation with exptl. data on metalloporphyrins  $\times$ -radical cations.  
 IT 120644-25-9 131214-86-3 144811-83-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (AM1 MO calcns. of, conformation in relation to)  
 RN 120644-25-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

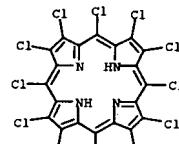
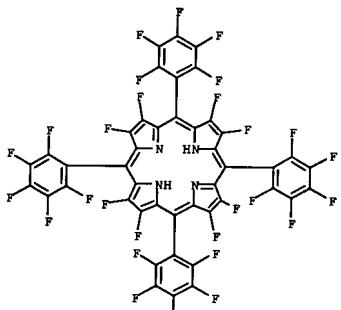
L6 ANSWER 129 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L6 ANSWER 130 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1993:6776 CAPLUS  
 DOCUMENT NUMBER: 118:6776  
 TITLE: Electronic effects of peripheral substituents in porphyrins: x-ray photoelectron spectroscopy and ab initio self-consistent field calculations  
 AUTHOR(S): Gassman, Paul G.; Ghosh, Abhik; Almlof, Jan  
 CORPORATE SOURCE: Dep. Chem., Univ. Minnesota, Minneapolis, MN, 55455, USA  
 SOURCE: Journal of the American Chemical Society (1992), 114(25), 9990-10000  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

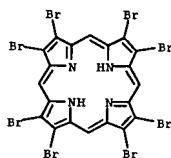
AB The electronic effects of a wide variety of peripheral substituents in free base porphyrins have been evaluated using XPS and all-electron ab initio calcns. Both methods have identified the 1s energies of the central N atoms as excellent sensors of the electronic effects of peripheral substituents. Core level photoelectron spectra are reported for nine porphyrins, including unsubstituted porphyrin, octaethylporphyrin, and seven tetraphenylporphyrins. Substituents on the Ph groups in tetraphenylporphyrins modulate the electronic environment of the central region of the porphyrin nucleus in a significant manner. Thus, between tetraphenylporphyrin and tetrakis(pentafluorophenyl)porphyrin, the XPS nitrogen 1s ionization potentials shift by 0.9 eV. Ab initio SCF calcns. were carried out on substituted porphyrins, with multiple alkyl, aryl, fluoro, chloro, bromo, cyano, and nitro groups, using basis sets of double- $\zeta$  quality. Calcns. on selected porphyrins with larger, polarized basis sets suggest that both the absolute values of the orbital energies and the substituent effects are reasonably well converged at the double- $\zeta$  level of basis sets. Very large substituent effects (<4.1 eV, relative to octamethylporphyrin) on the 1s energies of the central N atoms of the porphyrin nucleus are predicted for certain arrays of electron-withdrawing peripheral substituents. Valence orbital energies have also been computed, and the differences in the UV photoelectron spectra of porphyrin and octaalkylporphyrins are well reproduced by the calcns. Suitable arrays of strongly electron-withdrawing substituents result in large stabilizations of the porphyrin  $\pi$  orbitals, which should translate into enhanced stability of the porphyrin toward oxidative degradation. The mols. studied by the ab initio calcns. range in size from porphyrin, C20H14N4, to  $\beta$ -octafluoro-meso-tetrakis(pentafluorophenyl)porphyrin, C44H22F28N4. Use of the direct SCF formalism, in which integrals do not need to be stored, has made these large calcns. feasible. These calcns. demonstrate that at present ab initio calcns. can be performed routinely for mols. containing 50-100 atoms.

IT 121399-88-0 144811-81-4 144811-82-5  
 144811-83-6 144811-86-9 144811-87-0  
 144811-92-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (electronic effect of peripheral substituent in, MO calcn. of)  
 RN 121399-88-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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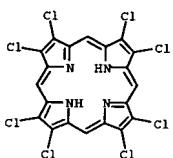


RN 144811-83-6 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)

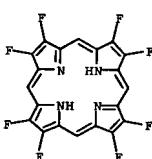


RN 144811-86-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)

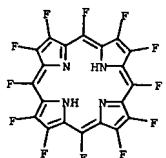
RN 144811-81-4 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)



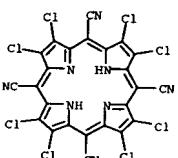
RN 144811-82-5 CAPLUS  
 CN 21H,23H-Porphine, 2,3,5,7,8,10,12,13,15,17,18,20-dodecachloro- (9CI) (CA INDEX NAME)



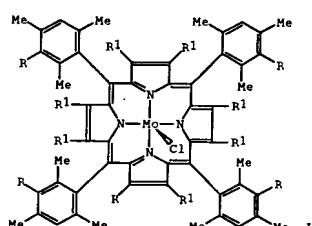
RN 144811-87-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,5,7,8,10,12,13,15,17,18,20-dodecafluoro- (9CI) (CA INDEX NAME)



RN 144811-92-7 CAPLUS  
 CN 21H,23H-Porphine-5,10,15,20-tetracarbonitrile, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)

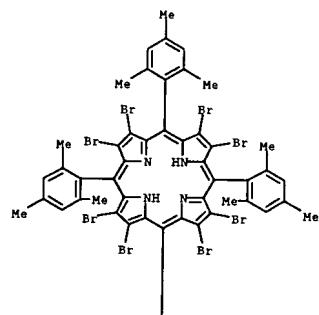


L6 ANSWER 131 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 1992:633728 CAPLUS  
 117:233728  
 ACCESSION NUMBER:  
 DOCUMENT NUMBER:  
 TITLE:  
 Preparation and catalytic activities of molybdenum  
 halogenated porphyrins in hydrogen peroxide olefin  
 oxidations  
 AUTHOR(S): Hoffmann, Pascal; Meunier, Bernard  
 CORPORATE SOURCE: Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.  
 SOURCE: New Journal of Chemistry (1992), 16(5), 559-61  
 DOCUMENT TYPE: CODEN: NJCHE5; ISSN: 0398-9836  
 LANGUAGE: Journal  
 OTHER SOURCE(S): English  
 GI CASREACT 117:233728

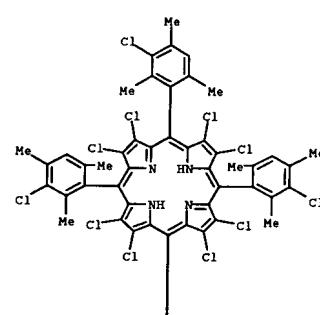


AB MoIII(Br8TMP)Cl (TMP = meso-tetramesitylporphyrinato) (I, R = H, R1 = Br) and MoIII(Cl12TMP)Cl (I, R = R1 = Cl) catalyze the epoxidn. of cyclooctene by 30% hydrogen peroxide in Et acetate at 70°. 129006-48-0  
 IT RL: RCT (Reactant); RACT (Reactant or reagent)  
 (metalation of, with molybdenum hexacarbonyl)  
 RN 129006-48-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

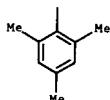
PAGE 1-A



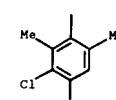
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IT 141573-97-9B  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and metalation of, with molybdenum hexacarbonyl)  
 RN 141573-97-9 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3-chloro-2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

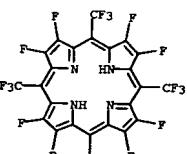
DOCUMENT NUMBER: 117:92626  
 TITLE: Metal coordination complex catalysts containing a halogenated ligand for hydrocarbon oxidation  
 INVENTOR(S): Ellis, Paul E., Jr.; Lyons, James E.; Myers, Harry K., Jr.  
 PATENT ASSIGNEE(S): Sun Refining and Marketing Co., USA  
 SOURCE: Eur. Pat. Appl., 7 pp.  
 CODEN: EPXADW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 11  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 471561	A2	19920219	EP 1991-307493	19910814
EP 471561	A3	19920226		
R: BE, DE, FR, GB, IT, NL NO 9103150 CA 0549177 JP 05138037 US 5663328	A AA A2 A	19920217 19920217 19930601 19970902	NO 1991-3150 CA 1991-2049177 JP 1991-229785 US 1996-672202	19910813 19910814 19910816 19960627

PRIORITY APPLN. INFO.: US 1990-568116 A 19900816  
 US 1987-246 A2 19870102  
 US 1987-66666 A2 19870626  
 US 1989-425089 B2 19891023  
 US 1994-303106 A3 19940907

OTHER SOURCE(S): MARPAT 117:92626  
 AB The catalysts, useful for oxidation of alkanes, are perhalogenated porphyrin or perhalogenated phthalocyanine metal complexes (metal = Fe, Cr, Mn, Ru, and /or Cu), and are used to catalyze air or O<sub>2</sub> oxidation of aliphatic hydrocarbons. Thus, air oxidation of isobutane in C6H<sub>6</sub> at 80° in presence of 0.013 mmol Fe(TPP2OBu<sub>8</sub>)Cl (TPP = tetraphenylporphyrin moiety) gave 8% mol tert-BuOH/100 mol liquid product and 3135 mol O<sub>2</sub> consumed/mol catalyst.

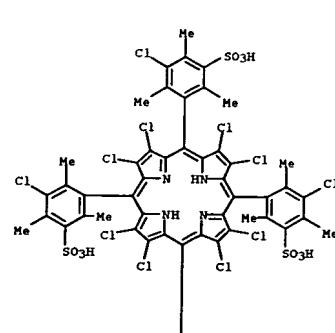
IT 142873-10-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with ferrous chloride)  
 RN 142873-10-7 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octtafluoro-5,10,15,20-tetrakis(trifluoromethyl)- (9CI) (CA INDEX NAME)



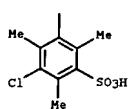
ACCESSION NUMBER: 1992:447538 CAPLUS  
 DOCUMENT NUMBER: 117:47538  
 TITLE: Olefin epoxidation and alkane hydroxylation catalyzed by robust sulfonated manganese and iron porphyrins supported on cationic ion-exchange resins  
 AUTHOR(S): Campestrini, Sandro; Meunier, Bernard  
 CORPORATE SOURCE: Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.  
 SOURCE: Inorganic Chemistry (1992), 31(11), 1999-2006  
 CODEN: INOCAJ, ISSN: 0020-1669

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 117:47538  
 AB Robust sulfonated manganese and iron porphyrins supported on poly(vinylpyridinium) polymers have been used as catalysts in olefin epoxidation, and alkane hydroxylation by iodosylbenzene. The metallocporphyrins are attached to protonated or methylated poly(vinylpyridine) polymers by the coordination of one pyridine unit, thus providing a proximal effect, and by addnl. interactions of the porphyrin sulfonato groups with the polymer pyridinium units. The best catalysts are the complexes containing halogen atoms at the pyrrole  $\beta$ -positions. In all these oxygenation reactions manganese porphyrins are better catalysts than the corresponding iron complexes. Comparative studies with another ion-exchange resin without a potential axial ligand show that the proximal effect is a key factor in metallocporphyrin-catalyzed reactions, not only for soluble complexes but also for supported catalysts.

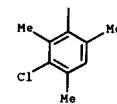
IT 142068-64-2  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and complexation with manganese)  
 RN 142068-64-2 CAPLUS  
 CN Benzenesulfonic acid, 3,3',3''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetra-5-chloro-2,4,6-trimethyl-, tetrasodium salt (9CI) (CA INDEX NAME)



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• 4 Na

IT 141573-97-9

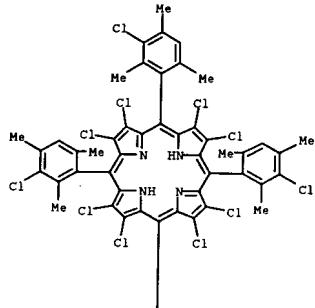
RL: RCT (Reactant); RACT (Reactant or reagent)

(sulfonation of)

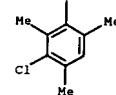
RN 141573-97-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3-chloro-2,4,6-trimethylphenyl)- (9Cl) (CA INDEX NAME)

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L6 ANSWER 134 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:434399 CAPLUS

DOCUMENT NUMBER: 117:34399

TITLE: Preparation and catalytic activity of the manganese(III) dodecachlorotetramesitylporphyrin complex

AUTHOR(S): Hoffmann, Pascal; Robert, Anne; Meunier, Bernard

Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.

CORPORATE SOURCE: Comptes Rendus de l'Academie des Sciences, Serie II:

Mecanique, Physique, Chimie, Sciences de la Terre et

de l'Univers (1992), 314(1), 51-6

SOURCE: CODEN: CRAMED; ISSN: 0764-4450

DOCUMENT TYPE: Journal

LANGUAGE: French

AB Chloration with N-chlorosuccinimide of the zinc complex of tetramesitylporphyrin gives, after demetalation, the free porphyrin ligand meso-tetrakis(3-chloro-2,4,6-trimethylphenyl)- $\beta$ -octachloroporphyrin, H<sub>2</sub>C<sub>12</sub>TMP. The manganese and iron complexes of this new halogenated porphyrin were prepared. The catalytic activity of Mn(C<sub>12</sub>TMP)Cl was evaluated and compared with the activities of Mn(TMP)Cl and Mn(Br<sub>8</sub>TMP)Cl, when these catalysts are associated with potassium monopersulfate or magnesium monoperphthalate as oxygen donors. An abridged English version is included.

IT 141573-97-9

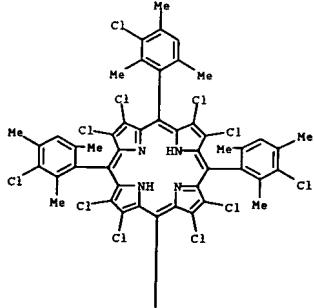
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(preparation and metalation of, in catalyst preparation)

RN 141573-97-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3-chloro-2,4,6-trimethylphenyl)- (9Cl) (CA INDEX NAME)

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L6 ANSWER 135 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1992:426161 CAPLUS  
DOCUMENT NUMBER: 117:26161

TITLE: Preparation and catalytic activities of the manganese and iron derivatives of Br8TMP and Cl12TMP, two robust porphyrin ligands obtained by halogenation of tetramesitylporphyrin

AUTHOR(S): Hoffmann, P.; Robert, A.; Meunier, B.  
CORPORATE SOURCE: Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.  
SOURCE: Bulletin de la Societe Chimique de France (1992), 129(1), 85-97

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The ionic halogenation of tetramesitylporphyrin by N-bromosuccinimide or N-chlorosuccinimide gives, as main product, meso-tetramesityl- $\beta$ -octabromoporphyrin (H2Br8TMP) and meso-tetrakis(3-chloro-2,4,6-trimethylphenyl)- $\beta$ -octachloroporphyrin (H2Cl12TMP), resp. Both Mn and Fe derivs. of these two porphyrins are efficient catalysts for olefin epoxidation and alkane hydroxylation. The kinetic isotope effects of hydroxylation reactions were determined using different porphyrin catalysts

and various O atom donors. The  $\Delta H/\Delta D$  values ranged from 2  $\pm$

0.8 to 9  $\pm$  3 and were more dependent on the nature of the central metal and the oxidant than on the structure of the porphyrin ligand itself. PhIO is the only O atom donor in association with Fe porphyrins able to give high kinetic isotope effects (7.7 to 9.0) close to the primary isotope effects reported for cytochrome P 450 itself.

IT 129006-48-0 P 141573-97-9

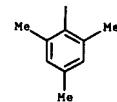
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and complexation of)

RN 129006-48-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

(Continued)

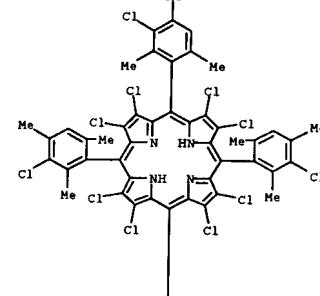


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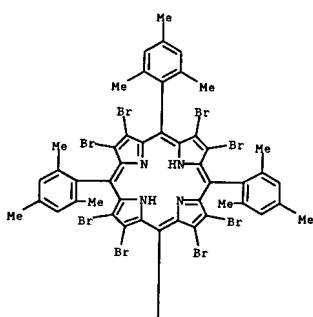
RN 141573-97-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3-chloro-2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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L6 ANSWER 136 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1992:247254 CAPLUS  
DOCUMENT NUMBER: 116:247254

TITLE:  $\beta$ -Halogenated-pyrrole porphyrins. Molecular

structures of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetramesitylporphyrin, nickel(II) 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrramesitylporphyrin, and nickel(II) 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin

AUTHOR(S): Mandon, D.; Ochenbein, P.; Fischer, J.; Weiss, R.; Jayaram, K.; Austin, R. N.; Gold, A.; White, P. S.; Brigaud, O.; et al.

CORPORATE SOURCE: Inst. Lebel, Univ. Louis Pasteur, Strasbourg, F-67070, Fr.

SOURCE: Inorganic Chemistry (1992), 31(11), 2044-9

CODEN: INOCAV; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The x-ray structures of the  $\beta$ -substituted-pyrrole tetraarylporphyrin 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetramesitylporphyrin (H2TMOBP), Ni(TMOBP), and Ni(TPFPBP-1/2CH2Cl2 (H2TPFPBP = 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin) are reported. The synthesis of H2TPFPBP is described. All these mols. are nonplanar, displaying saddle-shaped conformations. The saddle distortions minimize the intramol. steric interactions between the Br substituents and the ortho (ortho') C atoms or ortho (ortho') substituents of the Ph rings, and consequently, the corresponding contact distances have similar values in all compds. Because of the distortion of the porphyrin cores, the cavity defined by the ortho (ortho') substituents gives slightly less steric protection than in the nonbrominated nearly planar ortho- and ortho'-substituted tetraarylporphyrin complexes.

Crystalllog. data: H2TMOBP: tetragonal, space group P.hivin.421c, Z = 2, R = 0.054, R<sub>w</sub> = 0.069; Ni(TMOBP): tetragonal, space group P.hivin.421c, Z = 2, R = 0.049, R<sub>w</sub> = 0.057; Ni(TPFPBP-1/2CH2Cl2: monoclinic, space group C2/c, Z = 8, R = 0.047, R<sub>w</sub> = 0.064.

IT 129006-48-0

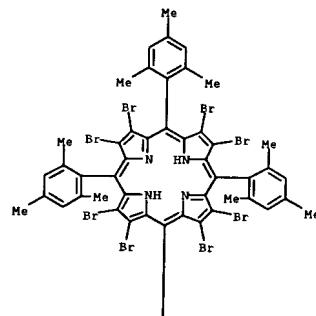
RL: RCT (Reactant); RACT (Reactant or reagent)  
(crystal structure and reaction of, with nickel acetate)

RN 129006-48-0 CAPLUS

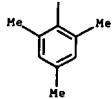
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 136 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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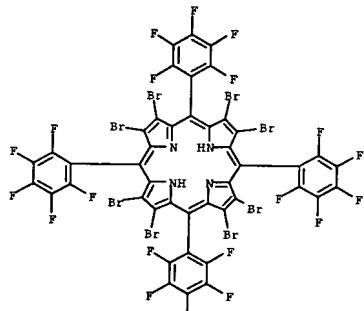
IT 139944-26-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with nickel acetate)

RN 139944-26-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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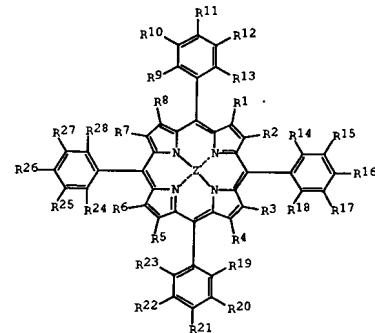
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L6 ANSWER 137 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 1992:213987 CAPLUS  
 116:213987  
 TITLE: Oxidation of olefins with oxygen catalyzed by halogenated porphyrin complexes  
 INVENTOR(S): Tsuchiya, Shinji; Kawai, Motomasu  
 PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.  
 CODEN: JKOKAF

DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03246238	A2	19911101	JP 1990-42342	19900226
JP 2790885	B2	19980827		

PRIORITY APPLN. INFO.: OTHER SOURCE(S): MARPAT 116:213987  
 GI



I

AB Olefinic compds. are oxidized with O to O-containing compds. in the presence of I [R1 - R28 = Cl-4 alkyl, trihalomethyl, H, halo;  $\geq 1$  of R1 - R28 is halo; Z consisting of a cation of a valence (M<sup>+</sup>) from Groups IA to VIA, IB to VIIIB, and VIII elements and an anion (X<sup>-</sup>) from O, F<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>, O<sup>-</sup>, OH<sup>-</sup>, MeO<sup>-</sup>, ETO<sup>-</sup>, PrO<sup>-</sup>, i-PrO<sup>-</sup>, PhO<sup>-</sup>, ACO<sup>-</sup>, CN<sup>-</sup>, CSN<sup>-</sup>, and ClO<sup>-</sup> in the form of 2M<sup>+</sup>, H<sup>+</sup>M<sup>+</sup>, M<sup>2+</sup>, M<sup>3+</sup>X<sup>-</sup>, M<sup>4+</sup>X<sup>-</sup>, OM<sup>4+</sup>, or OM<sup>5+</sup>X<sup>-</sup>; n = 1-5]. The reaction may be carried out in the presence of a base (for example, alc. and typically MeOH) and the process is applicable to propylene, 1-butene, 2-butene, butadiene, isoprene, cyclopentene,

L6 ANSWER 137 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
 cycloheptene, cyclooctene, 1,4-cyclooctadiene, styrene,  $\alpha$ -methylstyrene,  $\beta$ -methylstyrene, stilbene, allyl chloride, allyl bromide, allyl alc., oleic acid, and oleic acid esters. Thus, stirring 7 mmol cyclooctene with air at 25° in the presence of 1  $\mu$ mol 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrinatoiron (III) chloride gave 0.08 mmol 1,2-epoxycyclooctane vs. 0.01 mmol in the presence of tetrakis(2,4,6-trimethylphenyl)porphyrinatoiron (III).

IT 121399-88-02

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, with ferric chloride)

RN 121399-88-0 CAPLUS

CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9Cl) (CA INDEX NAME)

L6 ANSWER 138 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 1992:106069 CAPLUS  
 116:106069  
 TITLE: Porphyrin complexes as oxidation catalysts for olefins  
 INVENTOR(S): Tsuchiya, Shinji; Senoo, Manabu; Kawai, Motomasu  
 PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.  
 CODEN: JKOKAF

DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03232534	A2	19911016	JP 1990-27219	19900208

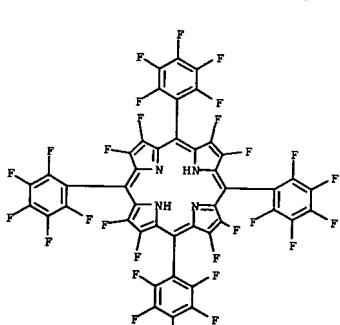
PRIORITY APPLN. INFO.: OTHER SOURCE(S): CASREACT 116:106069; MARPAT 116:106069

AB Epoxides and oxygen-containing compound were prepared by oxidation of olefins with oxygen in the presence of porphyrin complexes and alc<sub>2</sub>s or amines. Thus, air oxidation of 3 mmol cyclohexene in CH<sub>2</sub>Cl<sub>2</sub> in the presence of 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrinatoiron(III) chloride and MeOH at 25° for 2 h gave 0.15 mmol oxidation products 1,2-epoxycyclohexene, cyclohex-2-en-1-ol, and cyclohex-2-en-1-one in a ratio of 22:30:48.

IT 121399-88-02  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, with ferric chloride)

RN 121399-88-0 CAPLUS

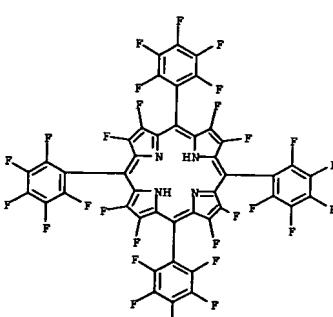
CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9Cl) (CA INDEX NAME)



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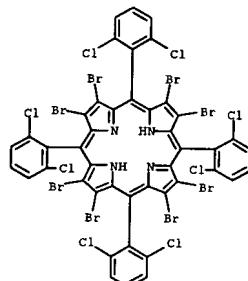
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L6 ANSWER 139 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1991:523796 CAPLUS  
 DOCUMENT NUMBER: 115:123796  
 TITLE: Silver halide color photographic material containing porphyrin for black spot prevention  
 INVENTOR(S): Kawasaki, Mikio  
 PATENT ASSIGNEE(S): Konica Co., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

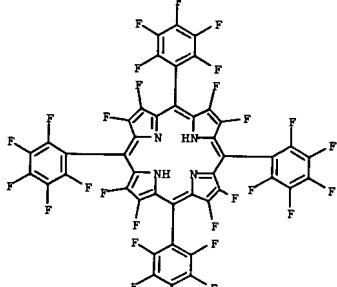
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03041441	A2	19910221	JP 1989-177732	19890707
PRIORITY APPLN. INFO.:		JP 1989-177732		19890707

OTHER SOURCE(S): MARPAT 115:123796  
 AB A photog. material contains  $\geq 1$  porphyrin derivative in the  $\pi$  hydrophilic layer on the support. It prevents the image layer from subjecting to generation of microspot defects, and is suitably applied to x-ray film for medical diagnosis.  $\alpha,\beta,\gamma,5$ -Tetraphenylporphyrin was added into the Ag(Br,I) emulsion for a black-and-white film for x-ray diagnosis.  
 IT 107035-95-0 121399-88-0 123762-91-3  
 RL: DEV (Device component use); USES (Uses)  
 (x-ray photog. film containing, for black spot prevention)  
 RN 107035-95-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

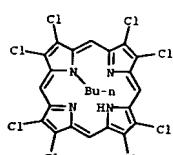


RN 121399-88-0 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

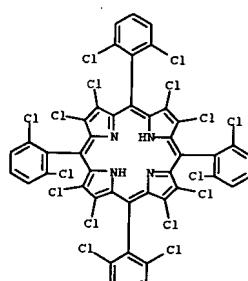
PAGE 1-A



RN 135762-91-3 CAPLUS  
 CN 21H,23H-Porphine, 21-butyl-2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)

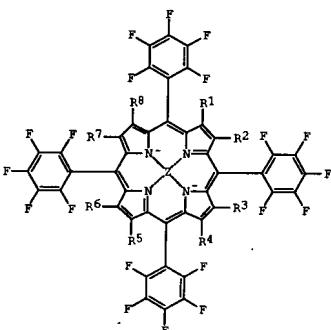


L6 ANSWER 140 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1991:514223 CAPLUS  
 DOCUMENT NUMBER: 115:114223  
 TITLE: Metal-assisted reactions. Part 22. Synthesis of perhalogenated porphyrins and their use as oxidation catalysts  
 AUTHOR(S): Gonsalves, Antonio M. D. Rocha; Johnstone, Robert A. W.; Pereira, Mariette M.; Shaw, Jacqueline; Sobral, Abilio J. F. do N.  
 CORPORATE SOURCE: Dep. Quim., Univ. Coimbra, Coimbra, 3000, Port.  
 SOURCE: Tetrahedron Letters (1991), 32(10), 1355-8  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB meso-Tetraarylporphyrins have been perchlorinated and perbrominated at peripheral (B) positions of the pyrrole rings by high-yielding procedures. These halogenated porphyrins show enhanced catalytic activity towards oxidation of alkanes and alkenes but are not stable when H<sub>2</sub>O<sub>2</sub> is used as the O donor. The reason for this instability appears to lie in excessive homolytic dissociation of H<sub>2</sub>O<sub>2</sub> with consequent rapid attack at the porphyrin B-position.  
 IT 134833-67-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and complexation of, with manganese)  
 RN 134833-67-3 CAPLUS  
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

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L6 ANSWER 141 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1991:479933 CAPLUS  
DOCUMENT NUMBER: 115:79933  
TITLE: Fluorine-substituted porphyrin complex for oxidation  
catalyst of organic compound  
INVENTOR(S): Tsucho, Shinji; Senoo, Manabu; Kawai, Motomasu  
PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
CODEN: JKOXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02250883	A2	19901008	JP 1989-241912	19890920
JP 2845982	B2	19990113		
PRIORITY APPLN. INFO.:			JP 1988-310051	A1 19881209
OTHER SOURCE(S):	MARPAT	115:79933		

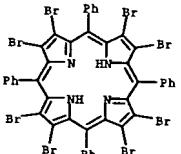


AB The complex is I [R1-R = H, F ( $\geq$ 1); Z = Group IA-VIA, cation ( $\geq$ 4); or Group IV-VIIIB, VIII, and anion ( $X^-$ ) O, F, Cl, Br, I, -, O-, OH-, OSO<sub>3</sub><sup>2-</sup>, Etc.], Me<sup>2</sup>CO, tert-BuO, PhO, AcO-, CN-, SCN-, and/or ClO<sub>4</sub><sup>-</sup> is possible form 2H<sub>2</sub>O, M<sup>2+</sup>, M<sub>3</sub>X<sup>+</sup>, M<sub>4</sub>X<sub>2</sub><sup>+</sup>, O<sub>2</sub>M<sup>2+</sup>X<sup>-</sup>. An organic compound is oxidized by peroxides with the complex as a catalyst. IT 12139-88-1

IT 121399-88-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of)

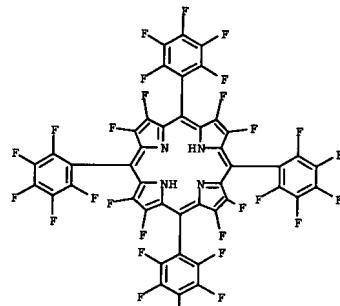
16 ANSWER 142 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN  
 ACCESSION NUMBER: 1991:54757 CAPLUS  
 DOCUMENT NUMBER: 114:54757  
 TITLE: Octabromotetraphenylporphyrin and its metal  
 derivatives: Electronic structure and electrochemical  
 properties  
 AUTHOR(S): Bhryappa, P.; Krishnan, V.  
 CORPORATE SOURCE: Dep. Inorg. Phys. Chem., Indian Inst. Sci., Bangalore,  
 560 012, India  
 SOURCE: Inorganic Chemistry (1991), 30(2), 239-45  
 CODEN: INCAJ; ISSN: 0020-1669  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Free-base octabromotetraphenylporphyrin (H2OBP) was prepared by bromination of Cu(TPP) (H2TPP = meso-tetraphenylporphyrin). M(OBr) (M = VO2+, Co, Ni, Cu, Zn, Pd, Ag, Pt) exhibit interesting electronic spectral features and electrochem. redox properties. The electron-withdrawing Br substituents at the pyrrole C atoms in H2OBP and M(OBr) produce remarkable red shifts in the Soret (50 nm) and visible bands (100 nm) of the porphyrin. The low magnitude of protonation consts. ( $pK_3 = 2.6$  and  $pK_4 = 1.75$ ) and the large red-shifted Soret and visible absorption bands make the octabromoporphyrin unique. The effect of electron-  
 Br substituents at the peripheral positions of the porphyrin was quant. analyzed by using the 4-orbital approach of M. J. Gouterman (1959). A comparison of MO parameters of M(OBr) with those of M(TPP) and M(Por) (H2Por = porphine) provides an explanation for the unusual spectral features. The Cl matrix element of M(OBr) is the lowest among the known substituted porphyrins, indicating delocalization of ring charge caused by the increase in conjugation of p orbitals of the Br onto the ring orbitals. The electron-transfer reactivities of the porphyrins are altered by the peripheral Br substituents, producing large anodic shifts in the ring and metal-centered redox potentials. The increase in anodic shift in the reduction potential

M(OBP) relative to M(TPP) is large (550 mV) compared to the shift in the oxidation potential (300 mV). These results were interpreted in terms of resonance and inductive interactions of the Br substituents.  
131214-86-3P  
RL: SPN (synthetic preparation); PREP (Preparation)  
(preparation and cyclic voltammetry and visible spectra and protonation  
131214-86-3 CAPLUS  
2H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-  
(9CI) (CA INDEX NAME)



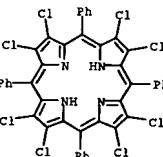
L6 ANSWER 141 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)  
RN 121399-98-0 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis[perfluorophenyl]- (SCI) (CA INDEX NAME)

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6 ANSWER 143 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1990:564403 CAPLUS  
 DOCUMENT NUMBER: 113:154403  
 TITLE: Highly chlorinated and perchlorinated  
 meso-tetraphenylporphyrins  
 AUTHOR(S): Wijesekera, Tilak; Matsumoto, Akiteru; Dolphin, David;  
 Lexa, Doris  
 CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T  
 1Y6, Can.  
 SOURCE: Angewandte Chemie (1990), 102(9), 1073-4  
 DOCUMENT TYPE: CODEN: ANCEAD; ISSN: 0044-8249  
 LANGUAGE: Journal  
 German  
 AB FeCl1 (H2L = meso-tetra(2,6-dichlorophenyl)porphyrin,  
 tetra(perchlorophenyl)porphyrin) were chlorinated by Cl2 gas in the  
 presence of FeCl13 in o-C6H4Cl2 to give FeL1Cl1 (H2L1 = meso-tetra(2,6-  
 dichlorophenyl)octachloroporphyrin, tetra(perchlorophenyl)octachloroporphyr-  
 yrin). Chlorination of Fe(TPP)Cl1 (H2TPP1 = tetraphenylporphyrin) by  
 Cl/FeCl3 led to decomposition of the macrocycle. Fe(TPP)Cl1 and H2TPP1 were  
 only partially chlorinated by N-chlorosuccinimide (I). Ni(TPP) reacted with I  
 in o-C6H4Cl2 to give NiL12 (H2L12 = octachloroporphyrin). Attempted  
 chlorination of M(TPP) (M = Cu, Zn) led to ring opening. The effect of  
 chlorination of the porphyrin coordinated to Fe was studied on the oxidative  
 and reduction potentials in the presence of Cl- and Ag+.  
 IT 120644-25-9P  
 RL: FORM (Formation, nonpreparative); PREP (Preparation)  
 (formation of, in demetalation of nickel complex)  
 RN 120644-25-9 CAPLUS  
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-  
 (9Cl) (CA INDEX NAME)

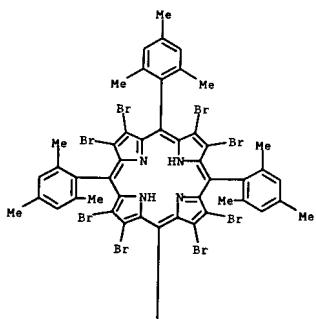


L6 ANSWER 144 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1990:514910 CAPLUS  
DOCUMENT NUMBER: 113:114910

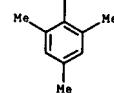
TITLE: Highly selective bromination of tetramesitylporphyrin: an easy access to robust metalloporphyrins, M-Br8TMP and M-Br8TPMS. Examples of application in catalytic oxygenation and oxidation reactions  
AUTHOR(S): Hoffmann, Pascal; Labat, Gilles; Robert, Anne; Meunier, Bernard  
CORPORATE SOURCE: Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.  
SOURCE: Tetrahedron Letters (1990), 31(14), 1991-4  
CODEN: TELEAY ISSN: 0040-4039

DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The N-bromosuccinimide bromination of the zinc derivative of meso-tetramesitylporphyrin, [Zn(TMP)], in MeOH under reflux in air, gives meso-tetramesityl- $\beta$ -octabromoporphyrinatozinc [Zn(Br8TMP)], in high yield (60-75%). Furthermore, the sulfonation by oleum of the metal-free ligand Br8TPMS gives meso-tetraakis(3,5-disulfonatomesityl)- $\beta$ -octabromoporphyrin, Br8TPMS2 (70-75%). These manganese and iron derivs., Mn(Br8TMP)Cl, Fe(Br8TMP)Cl, Mn(Br8TPMS), and Fe(Br8TPMS), are efficient catalysts in oxygen atom or electron transfer reactions.

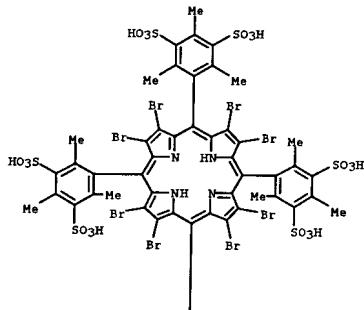
IT 129006-49-0P 129006-49-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and metalation of)  
RN 129006-49-0 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-(9CI) (CA INDEX NAME)



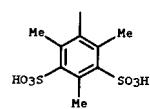
PAGE 1-A



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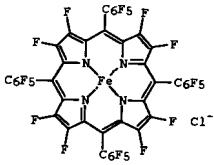
PAGE 1-A



PAGE 2-A

L6 ANSWER 145 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1989:457150 CAPLUS  
DOCUMENT NUMBER: 111:57150

TITLE: Novel synthetic method of phenol from benzene catalyzed by perfluorinated hemin  
AUTHOR(S): Tsuchiya, Shinji; Seno, Manabu  
CORPORATE SOURCE: Inst. Ind. Sci., Univ. Tokyo, Tokyo, 106, Japan  
SOURCE: Chemistry Letters (1989), (2), 263-6  
CODEN: CHLTAG ISSN: 0366-7022  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 111:57150  
GI



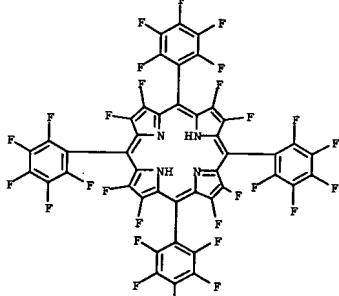
I

AB New perfluorinated hemin I catalyzes the hydroxylation of C6H6 by H2O2 at room temperature and 1 atm pressure. The turnover for PhOH produced in 2 h

IT 55. I also catalyzes the epoxidn. of cyclooctene by H2O2.  
121399-88-0  
RL: PROC (Process)  
(UV absorption of)  
RN 121399-88-0 CAPLUS  
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 145 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-A



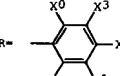
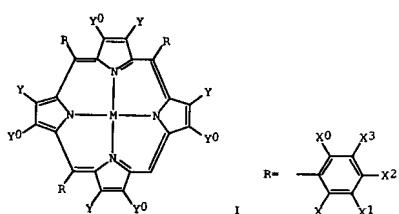
F

PAGE 2-A

L6 ANSWER 146 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1989:407144 CAPLUS  
 DOCUMENT NUMBER: 111:7144

TITLE: Metalated tetracyclic porphyrins, their nonmetalated precursors, and their use in the oxidation of lignin, alkanes, and alkenes  
 AUTHOR(S): Dolphin, David H.; Nakano, Taku; Kirk, Thomas Kent; Malone, Theodore E.; Farrell, Roberta L.; Wijesekera, Tilak Panini  
 PATENT ASSIGNEE(S): Can.  
 SOURCE: PCT Int. Appl., 46 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8807988	A1	19881020	WO 1988-US1240	19880415
WI: AU, DK, FI, JP, KR, NO, SU EV: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8817075	A1	19881104	AU 1988-17075	19880415
AU 617670	B2	19911205		
US 4892941	A	19900109	US 1988-181859	19880415
EP 363379	A1	19900418	EP 1988-904116	19880415
EP 363379	B1	19950614		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 02503086	T2	19900927	JP 1988-503781	19880415
CA 1308096	A1	19920929	CA 1988-564424	19880418
NO 8805571	A1	19890216	NO 1988-5571	19880415
DK 8807020	A	19881216	DK 1988-7020	19880415
KR 9702638	B1	19970307	KR 1988-71690	19880417
FI 92402	B	19940729	FI 1989-4898	19890106
FI 92402	C	19941110		
US 5077394	A	19911231	US 1989-455663	19891221
PRIORITY APPLN. INFO.:			US 1987-39566	A 19870417
			US 1988-181859	A3 19880415
OTHER SOURCE(S):	MARPAT	111:7144	WO 1988-US1240	A 19880415
GI				

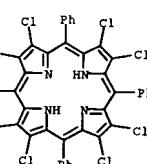


L6 ANSWER 146 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

AB Metalated porphyrins I [M = oxidation-sustaining transition metal, optionally with axial ligand; X, X0 = H, non-H2O-solubilizing electroneg. group; X1-X3 = H, electroneg. group; Y, Y0 = H, F, Cl; Z and/or Y0 = H when none of X1-X3 is H2O-solubles; 1-2 of X1-X3 is H2O-soluble and 2-2 of X's in non-H2O-soluble electroneg. group when Y = Y0 = H; 2-2 of X1-X3 is H2O-soluble] and their salt forms are prepared for use as oxidation catalysts, especially for oxidation-degradation of lignin in wood or pulp, hydroxylation of (cyclo)alkanes, and epoxidation of (cyclo)alkenes. Chlorination of chloro[meso-tetra-(2,6-dichlorophenyl)porphinato]iron(III) using FeCl3 and Cl at 140° gave 88% of the  $\beta$ -octachloro derivative, which underwent demetalation-sulfonation by fuming H2SO4 at 165° and metatalation by FeCl2.4H2O in DMF to give I (M = Fe with axial Cl ligand, X = Cl, X1 = X2 = H, X3 = SO3H, Y = Y0 = Cl) (II). Oxidation of 2 g northern softwood kraft by 0.5% (w/v) Me3COOH in buffer at pH 5 and 60° yielded a kappa value of 9.5 in the presence of 90 mg II, vs. 17.6 without II.

IT 120644-25-9P 120644-26-0P 120644-27-1P

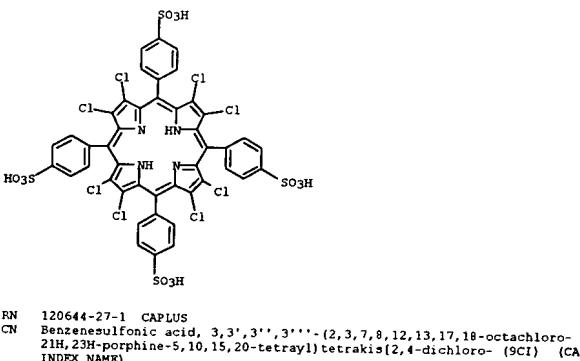
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and metatalation of)  
 RN 120644-25-9 CAPLUS  
 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetracyclic-(9Cl) (CA INDEX NAME)



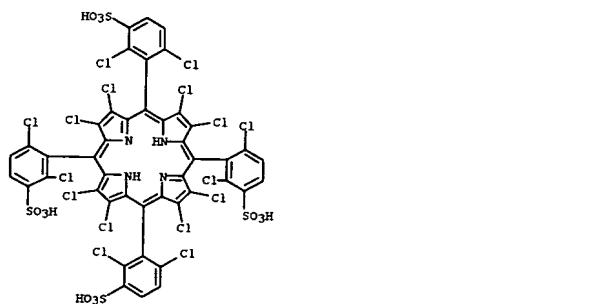
RN 120644-26-0 CAPLUS

CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis-(9Cl) (CA INDEX NAME)

L6 ANSWER 146 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 120644-27-1 CAPLUS  
 Benzenesulfonic acid, 3,3',3'',3'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetraakis[2,4-dichloro-(9Cl)] (CA INDEX NAME)



L6 ANSWER 147 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:107073 CAPLUS

DOCUMENT NUMBER: 110:107073  
 TITLE: Perhalogenated tetraphenylhemins: stable catalysts of high turnover catalytic hydroxylations [Erratum to document cited in CA106(18):148310d]  
 AUTHOR(S): Traylor, Teddy G.; Tsuchiya, Shinji  
 CORPORATE SOURCE: Dep. Chem., Univ. California, La Jolla, CA, 92093, USA  
 SOURCE: Inorganic Chemistry (1988), 27(24), 4520  
 CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

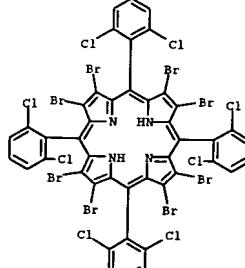
AB An error in Table I has been corrected. The error was not reflected in the abstract or the index entries.

IT 107035-95-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of (Erratum))

RN 107035-95-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)-(9Cl) (CA INDEX NAME)



ACCESSION NUMBER: 1987:148310 CAPIUS

DOCUMENT NUMBER: 106:148310

TITLE: Perhalogenated tetraphenylhemins: stable catalysts of high turnover catalytic hydroxylations

AUTHOR(S): Tsvetkov, Teddy G.; Tsuchiya, Shinji

CORPORATE SOURCE: Dep. Chem., Univ. California, La Jolla, CA, 92093, USA

SOURCE: Inorganic Chemistry (1987), 26(8), 1338-9

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Bromination of tetrakis(2,6-dichlorophenyl)porphyrinatozinc affords the 2,3,7,8,12,13,17,18-octabromo compound (48%) which is converted into FeLCl. This heme catalysts high turnover, rapid hydroxylation of alkanes without catalyst destruction.

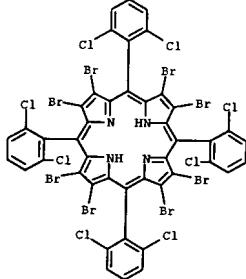
IT 107035-95-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 107035-95-0 CAPIUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-108.04	-108.04

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